

The Synthesis and Base-Induced Breakdown of Triaryl 1,4-Oxathiins. An Experimental and DFT Study.

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Mills and Adrian L. Schwan***

Supplementary Materials

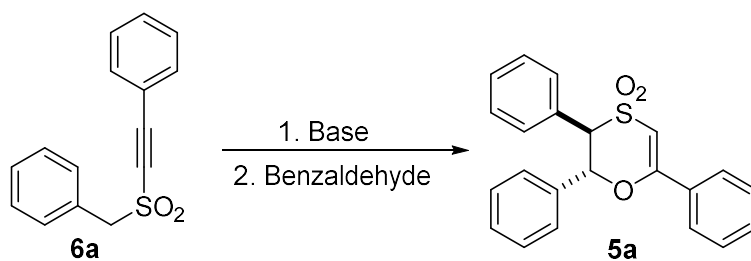
Tables relating to cyclization reaction optimization	S2
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Table S1. The effect of time on the production of product, by-product, starting material recovery and overall mass.

Time of reaction	Equivalency of			Mass recovery
	Starting material remaining	Oxathiin-S,S-dioxide (5a) ^a	By-product (7)	
45 min	2.0	1.0	0	84%
4 hours	0.8	1.0	0.12	70%
6 hours	0.3	1.0	0.26	63%
18 hours	0.1	1.0	0.35	52%
4 days	0	0	0	0%

^a Relative amount of oxathiin arbitrarily set to 1

Table S2: Optimizations for oxathiin formation



Entry	Base	Equivalents	Aldehyde equivalents	Isolated yield (%) ^a
1	BuLi	1.0	2.0	58
2	BuLi	0.7	2.0	23
3	BuLi	0.6	2.0	50
4	BuLi	0.45	2.0	57
5	BuLi	0.4	2.0	12
6	BuLi	0.25	2.0	19
7	BuLi	0.5	2.0	70
8	LDA	0.5	2.0	68
9	tBuOK	1.2	2.0	38
10	tBuOK	1.2	Xs	~5 (NMR)
12	NaH	1.2	2.0	~5 (NMR)
13	BuLi	0.5	1.5	72-76 ^b
14	LDA	0.5	1.5	58

^a Isolated yield unless indicated otherwise. ^b Multiple trials

Table S3. Ring openings of oxathiin **5a**

#	Base ^a	conditions	Extent of reaction ^b	Isolated yield	E/Z ratio ^c
1	LiOMe (1M in MeOH)	-35 °C/ 24 h	0%	--	--
2	NaOH (1M in MeOH)	-35 °C/ 24 h	90%	73%	10/90
3	KOtBu	-35 °C/ 24 h	68%	67%	22/78
4	LiOMe (1M in MeOH)	-35 °C/3 h; then rt/21 h	100%	82%	18/82
5	NaOH (1M in MeOH)	-35 °C/3 h; then rt/21 h	94%	75%	8/92
6	KOtBu	-35 °C/3 h; then rt/21 h	100%	87%	12/88
7	LiOMe (1M in MeOH)	rt/24 h	100%	83%	18/82
8	NaOH (1M in MeOH)	rt/24 h	95%	76%	8/92
9	KOtBu	rt/24 h	100%	90%	15/75
10	KOH (1M in MeOH)	rt/24 h	96%	81%	7/93
11	DBU	rt/24 h	100%	96%	17/83 ^d

a Reactions were performed in THF; Some bases were introduced via a 1 molar MeOH solution.

b Estimated by inspection of the ¹H NMR of the crude reaction mixture.

c Determined by ¹H NMR.

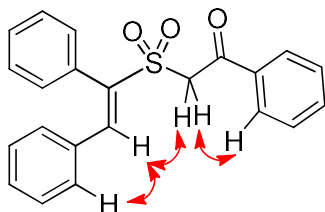
d Extended exposure created additional E isomer.

nOe Experiments of Keto-sulfones **7E**/**7Z**

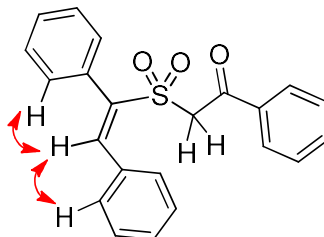
The 3D ^{13}C -NOESYHSQC spectrum was collected on a Bruker AVANCE III 600 MHz spectrometer equipped with a 5 mm TCI cryoprobe. The sample temperature was regulated at 298 ± 1 K. The pulse sequence *noesyhsqcetgp3d* was used as provided by Bruker. The NOESY mixing time was set to 500 ms, the interscan delay was set to 2.5 sec, and 8 scans were collected per increment.

Two approaches were utilized to optimize spectral resolution while minimizing spectrometer time. First: the ^{13}C dimension was collected with a spectral width of 9 ppm (centred at 131 ppm) which resulted in the aliasing of peaks associated with the vinyl C-H and CH_2 groups. The spectral width and central frequency were optimized to ensure the aliased peaks did not interfere with any other peaks. Second: the non-uniform sampling (NUS) feature of the Bruker Topspin acquisition software was used to randomly acquire 1792 increments from a conventional sampling grid of 36 indirect ^{13}C increments and 384 indirect ^1H increments (spanning 8.5 ppm), representing a NUS percentage of 13%. The total acquisition time was 12.74 h, as compared to > 98 h for a conventionally acquired spectrum. The spectrum was processed using the SMILE¹ NUS processing plug-in to the NMRPipe² processing suite.

Relevant nOe enhancements of **7E**:



Relevant nOe enhancements of **7Z**:



¹ J. Ying, F. Delaglio, D.A. Torchia, and A. Bax: Sparse Multidimensional Iterative Lineshape-Enhanced (SMILE) Reconstruction of Both Non-Uniformly Sampled and Conventional NMR Data. *J Biomol NMR* 68, 101-118 (2017).

² Delaglio F, Grzesiek S, Vuister GW, Zhu G, Pfeifer J, Bax A: NMRpipe—a multidimensional spectral processing system based on UNIX pipes. *J Biomol NMR* 6:277–293 (1995).

Figure S1. Optimized geometries of pre-complexes for addition of benzaldehyde to lithiated sulfone **8**.

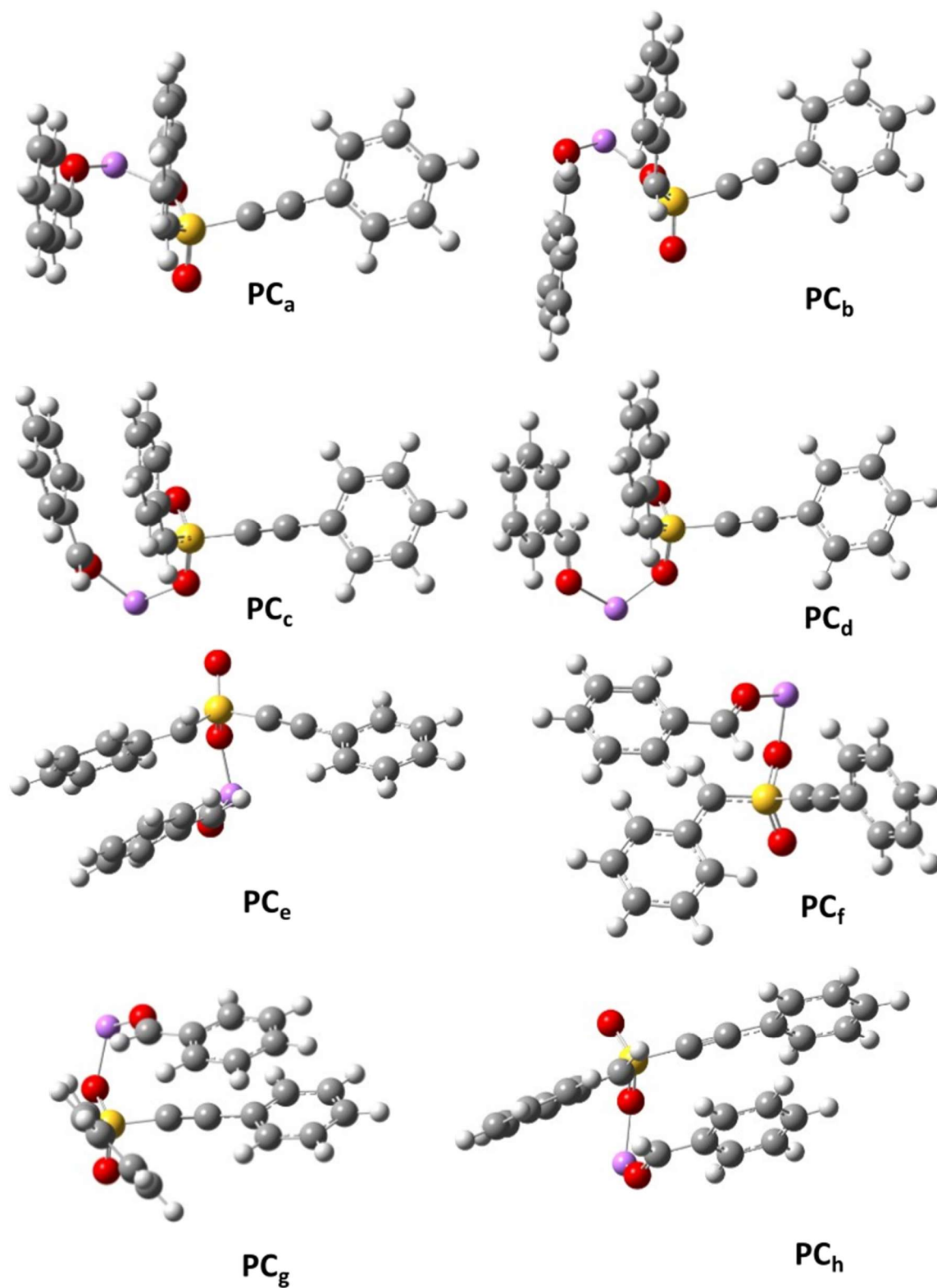


Figure S2: Optimized transition state structures for addition of benzaldehyde to lithiated sulfone **8**.

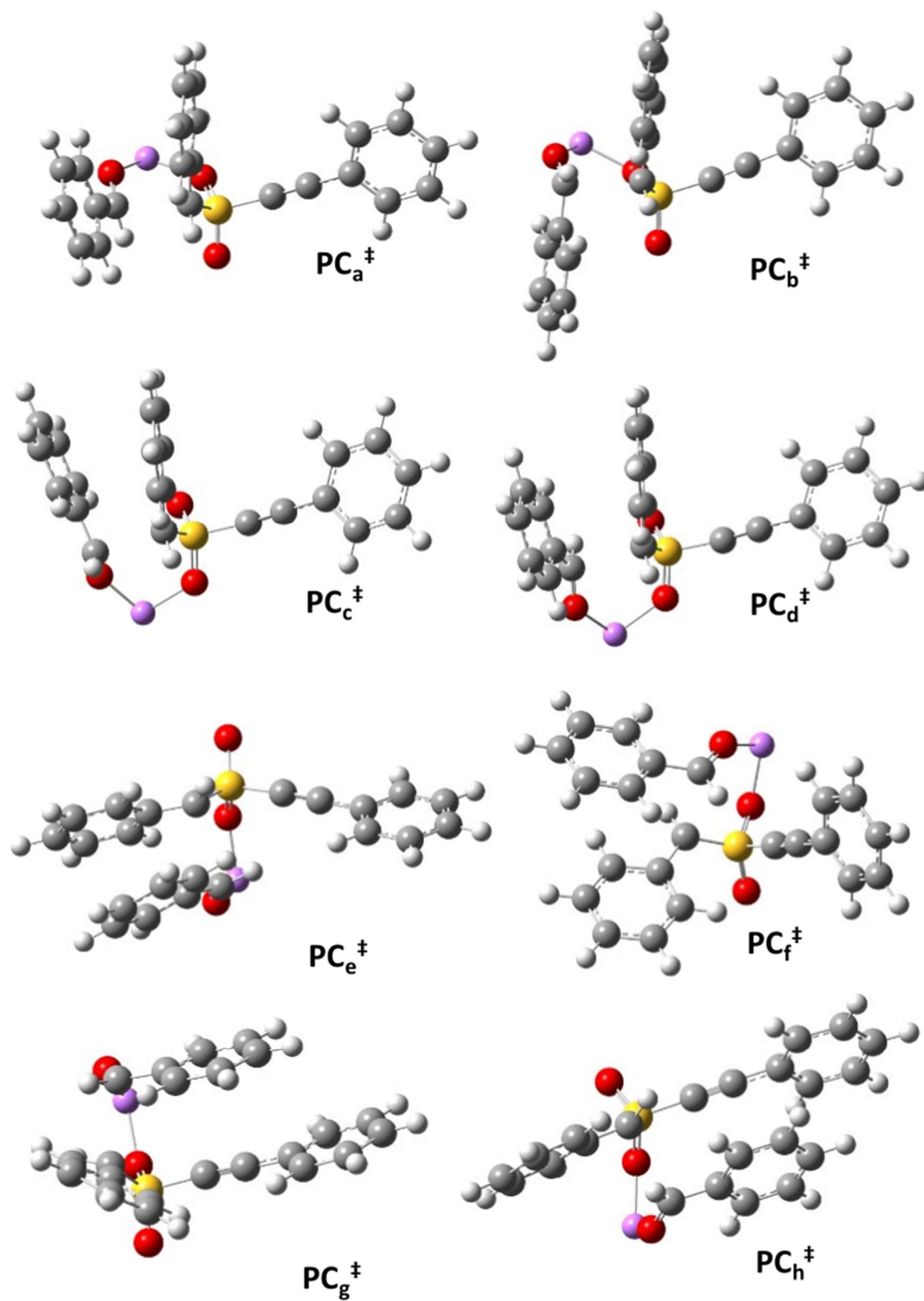


Figure S3. Optimized geometries of benzaldehyde addition products **9_{a-h}**

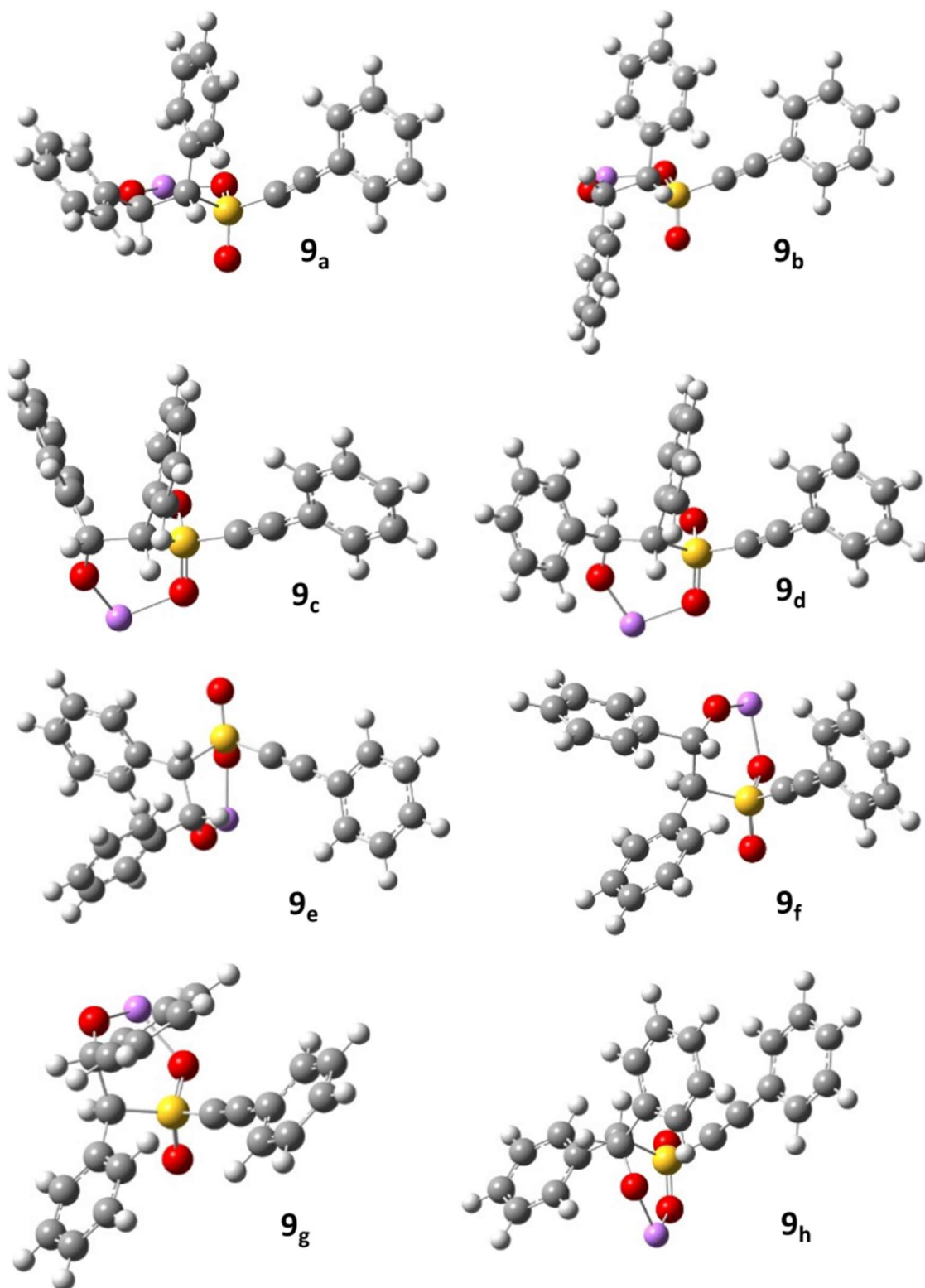


Figure S4. Energy profile for benzaldehyde addition to lithiated benzyl alkynyl sulfones. Reactions originate in the center and proceed left for cis cyclizations and right for trans cyclizations.

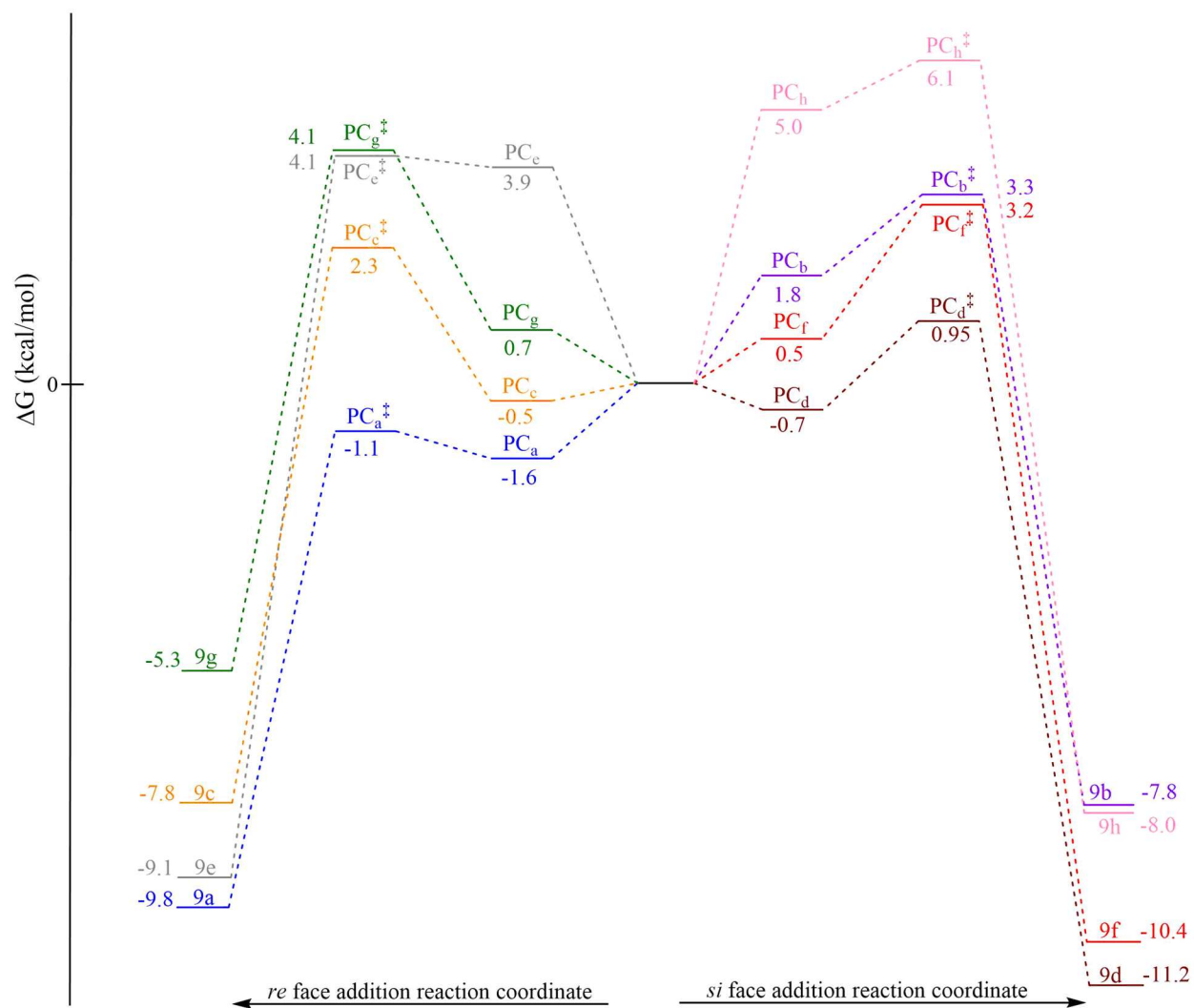


Table S4. Selected computed parameters for addition of benzaldehyde to lithiated sulfone **8**.

	C ₅ -C ₆ (Å)	C ₅ -S (Å)	S-O ₁ (Å)	S-O ₂ (Å)	S-C ₃ (Å)	C ₂ -C ₃ (Å)	C ₂ -O _b (Å)	O ₁ -Li (Å)	O ₂ -Li (Å)	O _b -Li (Å)	PhC ₃ -C ₂ Ph dihedral (°)	HC ₃ -C ₂ H dihedral (°)
PC_a	1.209	1.754	1.490	1.467	1.661	2.876	1.223	1.875	-	1.918	-52.1	-48.6
PC_b	1.209	1.754	1.490	1.464	1.659	2.801	1.222	1.882	-	1.921	-172.3	64.3
PC_c	1.209	1.757	1.467	1.490	1.657	2.856	1.225	-	1.901	1.932	15.7	22.2
PC_d	1.209	1.754	1.469	1.490	1.654	2.826	1.226	-	1.889	1.948	-27.1	-150.5
PC_e	1.207	1.738	1.471	1.491	1.673	2.755	1.226	-	1.898	1.921	-53.3	-49.0
PC_f	1.209	1.758	1.491	1.467	1.651	2.889	1.222	1.916	-	1.937	-56.9	177.7
PC_g	1.209	1.754	1.493	1.467	1.656	3.165	1.220	1.916	-	1.937	35.6	59.9
PC_h	1.206	1.729	1.473	1.495	1.679	2.706	1.225	-	1.883	1.908	-170.0	65.9
PC_a[‡]	1.208	1.743	1.486	1.464	1.683	2.419	1.239	1.903	-	1.885	-62.2	-55.7
PC_b[‡]	1.208	1.745	1.486	1.461	1.684	2.407	1.237	1.904	-	1.876	-169.8	65.5
PC_c[‡]	1.208	1.741	1.462	1.484	1.696	2.311	1.248	-	1.920	1.864	24.7	32.8
PC_d[‡]	1.209	1.743	1.465	1.485	1.683	2.394	1.242	-	1.921	1.893	-37.3	-161.5
PC_e[‡]	1.207	1.736	1.470	1.489	1.684	2.573	1.232	-	1.902	1.908	-54.1	-48.7
PC_f[‡]	1.207	1.741	1.487	1.465	1.684	2.449	1.238	1.933	-	1.880	-56.5	179.1
PC_g[‡]	1.206	1.730	1.488	1.467	1.690	2.399	1.241	1.905	-	1.877	64.9	69.3
PC_h[‡]	1.206	1.728	1.472	1.493	1.687	2.569	1.230	-	1.890	1.895	-169.1	66.5
9_a	1.206	1.718	1.473	1.457	1.816	1.585	1.351	1.994	-	1.785	-56.8	-42.2
9_b	1.206	1.721	1.473	1.455	1.824	1.584	1.352	1.988	-	1.772	-150.3	86.6
9_c	1.206	1.722	1.456	1.474	1.823	1.590	1.350	-	1.983	1.771	43.6	55.6
9_d	1.206	1.720	1.458	1.474	1.823	1.575	1.353	-	1.991	1.777	-59.8	179.2
9_e	1.206	1.717	1.457	1.473	1.819	1.577	1.353	-	1.971	1.783	-55.0	-39.2
9_f	1.206	1.718	1.473	1.456	1.823	1.577	1.351	1.978	-	1.775	-61.0	176.4
9_g	1.205	1.715	1.472	1.457	1.815	1.592	1.352	1.964	-	1.780	68.5	76.4
9_h	1.206	1.711	1.458	1.472	1.825	1.576	1.353	-	1.963	1.772	-150.9	84.7

Brief Discussion of Trends exhibited in Table S4.

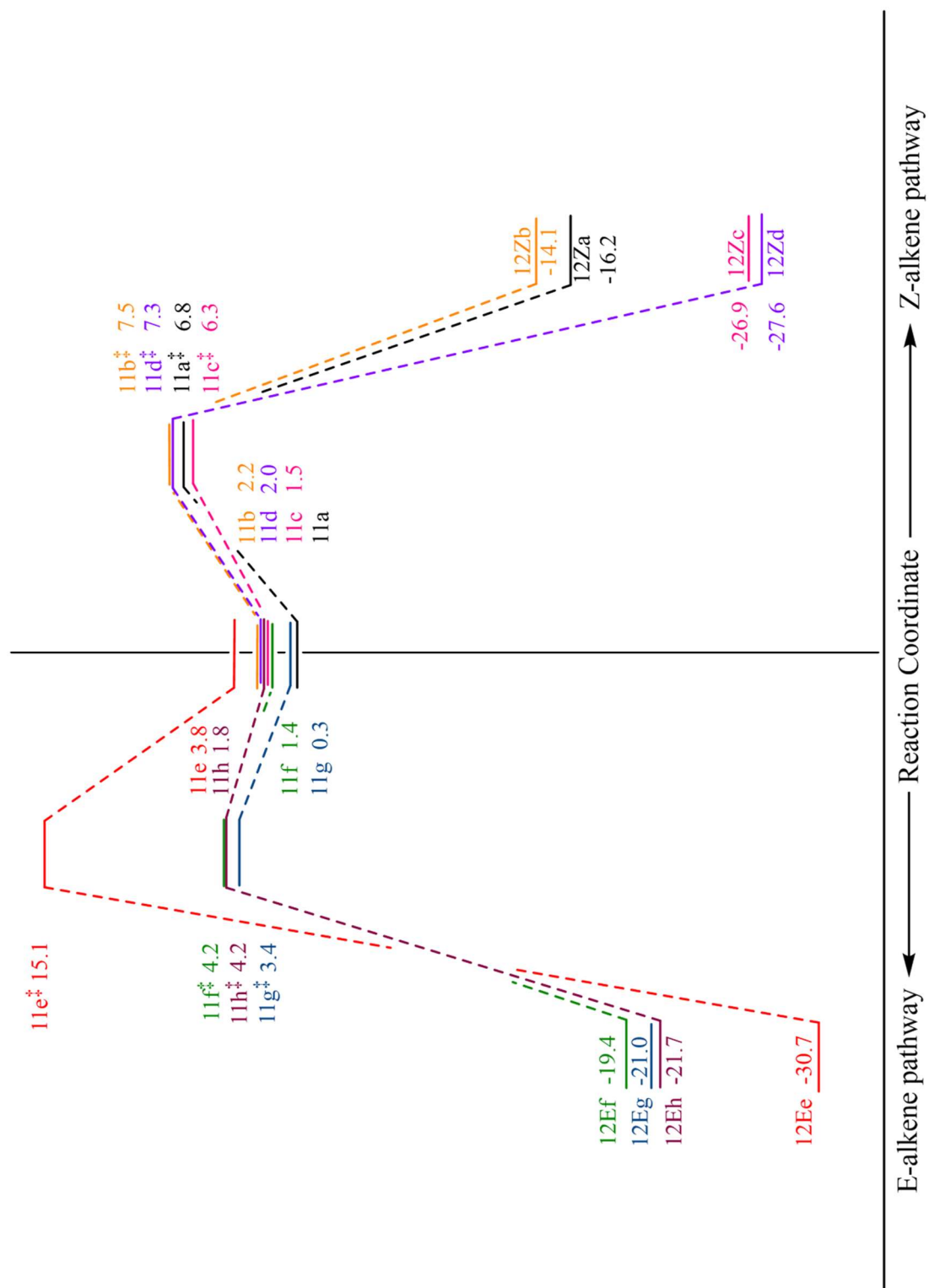
Pre-complexes contain similar bond lengths throughout the structures aside from C₂-C₃ distances, which vary from 2.706 Å in **PC_h** to 3.165 Å in **PC_g**. Regarding geometries for transition states of benzaldehyde addition, notable changes in bond length occur between C₂ and C₃ as formation of the bond progresses. The most significant change is observed in **PC_g[‡]** where the distance shortens by 0.766 Å, while the least significant change occurs in **PC_h[‡]** where the separation decreases by 0.137 Å. These systems have the highest energy transition states of their respective pathways, either due to the higher energy of the initial pre-complex (**PC_h**), or as a result of larger activation energies (**PC_g**). In conjunction with C₂-C₃ bond formation, a slight lengthening of both the S-C₃ and C₂-O_b bonds arises as the O_b-Li distance decreases.

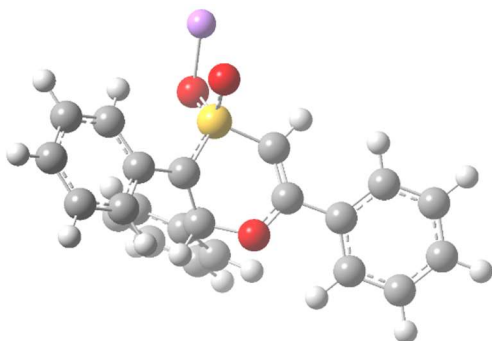
Transition states for benzaldehyde addition closely resemble the pre-complexes as evidenced by the low activation barriers and bond length data. Aside from the **PC_g/9_g** system, >60% of the closure of the C₂-C₃ interatomic distances occurs from transition state to product. The addition products **9** exhibit a slightly longer than average C-C bond length of 1.575-1.592 Å, in addition to elongated C₃-S (~0.16 Å) and C₂-O_b (~0.13 Å) bond distances. As the reaction progresses and the negative charge is transferred to O_b, there is an average decrease in the O_b-Li distance by 0.15 Å. The O₁ and O₂ to Li distances show minor increases as the counterion moves closer to the O_b oxyanion with elongations ranging from 0.05 – 0.12 Å.

Table S5. Bond lengths and angles for selected benzaldehyde addition products and pre-cyclization structures.

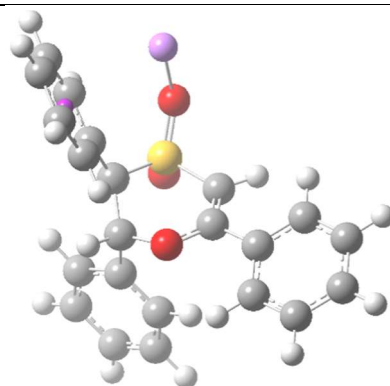
	C ₅ -C ₆ (Å)	C ₅ -S (Å)	S-O ₁ (Å)	S-O ₂ (Å)	S-C ₃ (Å)	C ₃ -C ₂ (Å)	C ₂ -O _b (Å)	O ₁ -Li (Å)	O ₂ -Li (Å)	O _b -Li (Å)	PhC ₃ -C ₂ Ph dihedral (°)	HC ₃ -C ₂ H dihedral (°)
9_g	1.205	1.715	1.472	1.457	1.815	1.592	1.352	1.964	-	1.780	68.5	76.4
9_e /9_{cis}	1.206	1.717	1.457	1.473	1.819	1.577	1.353	-	1.971	1.783	-55.0	-39.2
9_f	1.206	1.718	1.473	1.456	1.823	1.577	1.351	1.978	-	1.775	-61.0	176.4
9_h	1.206	1.711	1.458	1.472	1.825	1.576	1.353	-	1.963	1.772	-150.9	84.7
9_{trans}	1.206	1.718	1.473	1.456	1.822	1.577	1.351	1.979	-	1.774	-60.8	176.5

Figure S5. Energy profiles of ring opening of lithiated oxathiins.

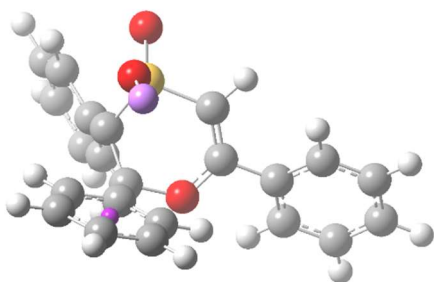




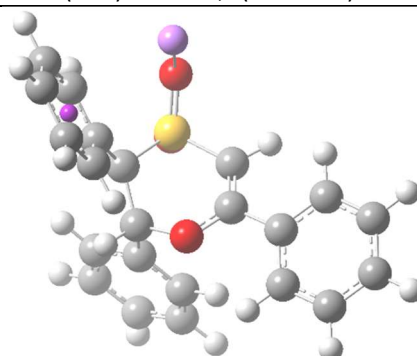
11a: $r(\text{Li-O}) = 1.989, 2.006 \text{ \AA}$



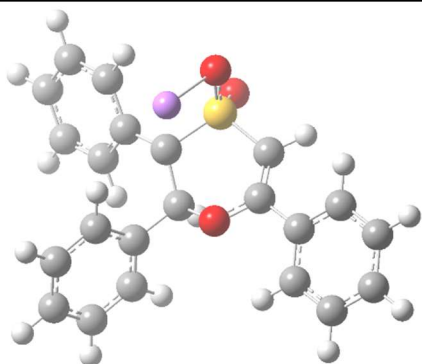
11b: $r(\text{Li-O}): 1.847 \text{ \AA}; r(\text{Li to 3-Ar}) = 3.257 \text{ \AA}$



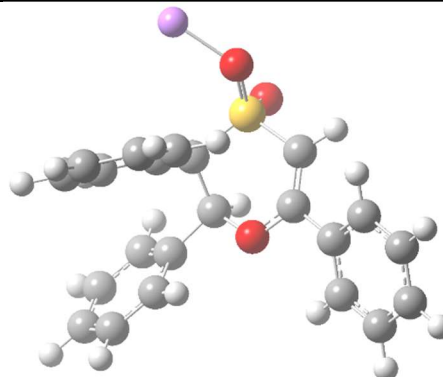
11c: $r(\text{Li-O}): 1.831 \text{ \AA}; r(\text{Li to 2-Ar}) = 3.119 \text{ \AA}$



11d: $r(\text{Li-O}): 1.857 \text{ \AA}; r(\text{Li to 3-Ar}) = 3.257 \text{ \AA}$



11e: $r(\text{Li-O}): 1.981 \text{ \AA}; r(\text{Li-C}): 2.339 \text{ \AA}$



11f: $r(\text{Li-O}): 1.869 \text{ \AA}; r(\text{Li-C}): 3.462 \text{ \AA}$

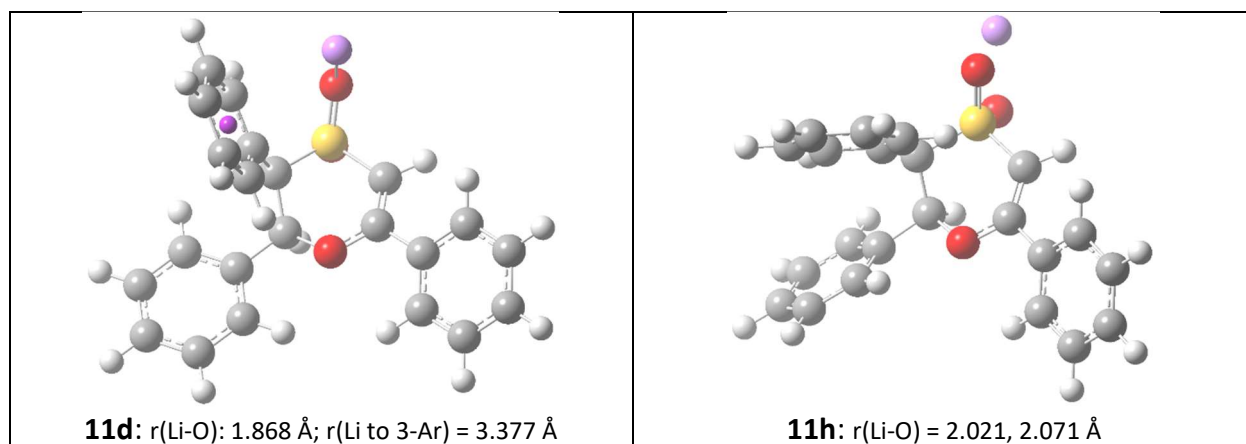


Figure S6 Optimized oxathiins 11 monolithated at carbon-3.

Comments about lithiated ring opening precursors 11 (Figure S6) :

1. Only structures **11a -11d** underwent ring opening to the kinetic product.
2. Structure **11b** and **11d** are very similar in geometry and energy.
3. Structures **11b**, **11c** and **11d** exhibit a strong Li to Ar interaction. Structure **11c** engages the Li with the Ph group on the 2-carbon of the ring, whereas structures **11b** and **11d** demonstrate a Li interaction with the Ph group on the 3-carbon of the ring.
4. Only structures **11a** and **11h** exhibit the lithium bridging between the two sulfonyl oxygens.
5. All eight of the structures (Figure S6) exhibit at least one strong sulfonyl O to Li affiliation (1.831 to 2.021 Å)
6. Structure **11e** holds the Li closest to the ‘deprotonated’ carbon (2.339 Å)

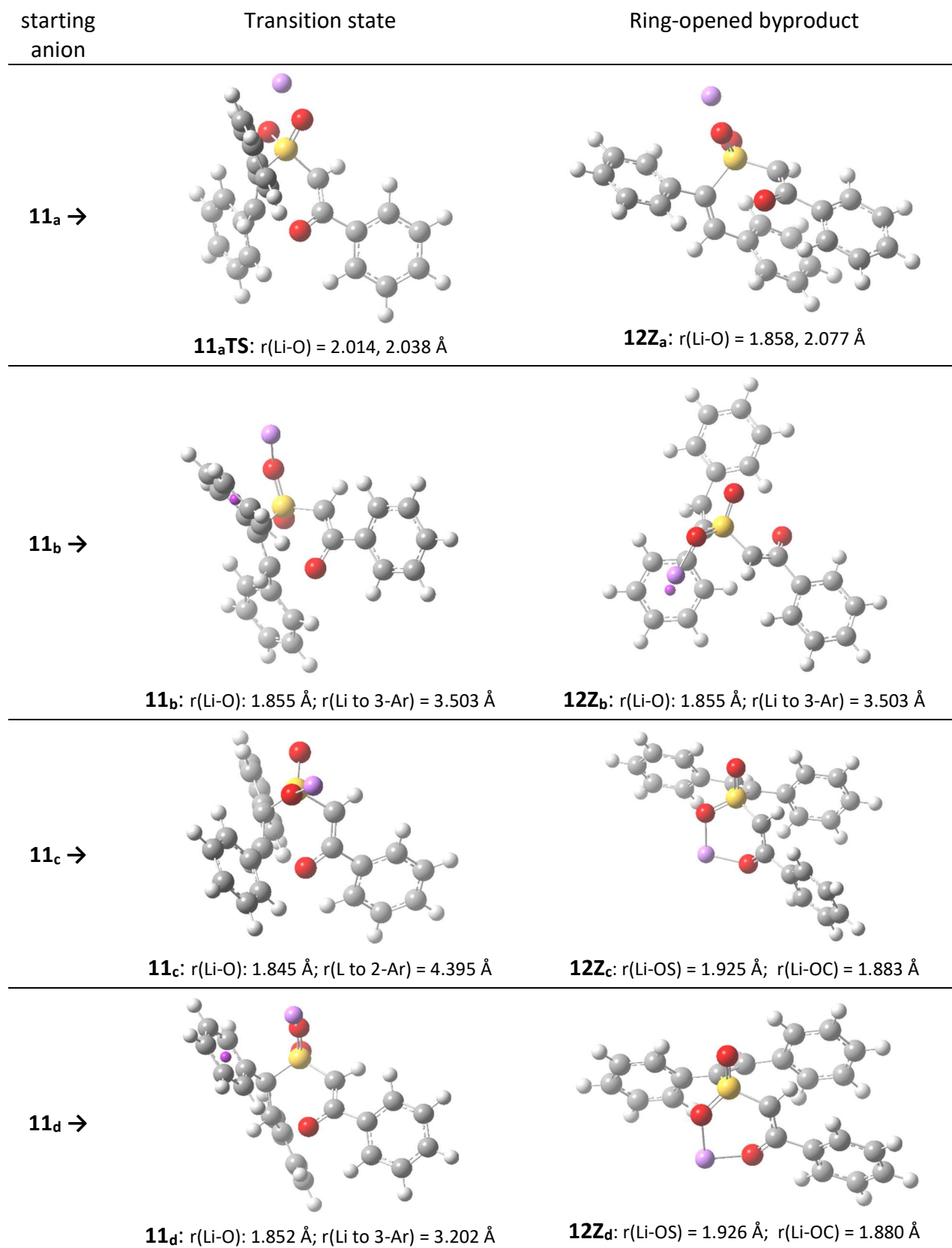


Figure S7 Optimized structures through ring opening for lithated substrates **11_{a-d}**.

Table S6. Bond lengths and angles of optimized geometries for the oxathiin ring opening process.

	C5-C6 (Å)	C5-S (Å)	S-O1 (Å)	S-O2 (Å)	S-C3 (Å)	C3-C2 (Å)	C2-Ob (Å)	O1-Li (Å)	O2-Li (Å)	Ob-Li (Å)	Ob-C6 (Å)	PhC3-C2Ph dihedral	Li-Ph centroid (Å)
11a	1.348	1.745	1.508	1.517	1.663	1.497	1.450	2.005	1.989	-	1.339	100.4	
11b	1.349	1.757	1.499	1.471	1.698	1.490	1.472	1.847	-	1.847	1.340	152.8	
11c	1.350	1.757	1.497	1.471	1.697	1.491	1.474	1.831	-	4.768	1.340	-155.7	
11d	1.349	1.757	1.500	1.471	1.698	1.489	1.473	1.857	-	4.854	1.340	153.4	
11e	1.343	1.750	1.508	1.476	1.731	1.516	1.458	1.981	-	3.477	1.341	-55.6	
11f	1.352	1.753	1.498	1.475	1.699	1.498	1.487	1.869	-	-	1.338	55.1	
11g	1.351	1.761	1.497	1.472	1.700	1.487	1.483	1.868	-	5.007	1.338	53.7	
11h	1.355	1.747	1.495	1.501	1.688	1.496	1.486	2.071	2.021	-	1.334	54.5	
11a‡	1.384	1.715	1.501	1.503	1.731	1.394	1.890	2.038	2.014	-	1.282	158.5	
11b‡	1.373	1.733	1.497	1.468	1.734	1.406	1.838	1.855	-	5.418	1.294	160.4	
11c‡	1.373	1.736	1.492	1.470	1.728	1.414	1.799	1.845	-	4.730	1.299	-158.1	
11d‡	1.378	1.730	1.501	1.472	1.744	1.394	1.889	1.852	-	4.757	1.288	160.7	
11e‡	1.349	1.764	1.513	1.470	1.718	1.443	1.733	1.940	-	2.113	1.347	-8.8	
11f‡	1.372	1.730	1.497	1.475	1.725	1.411	1.790	1.866	-	-	1.300	33.5	
11g‡	1.374	1.735	1.497	1.471	1.732	1.405	1.820	1.874	-	5.198	1.296	42.1	
11h‡	1.378	1.720	1.494	1.502	1.717	1.409	1.791	2.078	2.020	-	1.293	33.4	
12Za	1.412	1.683	1.491	1.498	1.814	1.335	3.335	2.076	2.066	-	1.243	178.3	
12Zb	1.402	1.698	1.499	1.463	1.808	1.337	3.623	1.858	-	-	1.248	-179.1	
12Zc	1.389	1.707	1.487	1.469	1.819	1.337	3.962	1.925	-	1.883	1.269	-176.2	
12Zd	1.390	1.702	1.490	1.468	1.822	1.336	3.677	1.926	-	1.879	1.268	178.8	
12Ee	1.392	1.704	1.491	1.467	1.807	1.336	3.654	1.913	-	1.862	1.265	-5.1	
12Ef	1.406	1.695	1.496	1.468	1.804	1.336	3.251	1.853	-	-	1.245	-4.1	
12Eg	1.405	1.698	1.498	1.467	1.801	1.335	3.317	1.855	-	-	1.246	4.2	
12Eh	1.408	1.685	1.496	1.494	1.799	1.335	3.461	2.093	2.035	-	1.245	6.4	

Table S7. Reaction free energies for proton transfers between possible anionic intermediates.

reactants	products	ΔG_r
10_{trans}' + 6	5_{trans} + 8c	-1.7
10_{trans}' + 5_{trans}	5_{trans} + 11c	2.7
10_{trans}' + 5_{cis}	5_{trans} + 11a	-3.3
10_{trans}' + 5_{cis}	5_{trans} + 11b	-1.1
10_{trans}' + 5_{cis}	5_{trans} + 11d	-1.3
10_{cis}' + 6	5_{cis} + 8c	2.8
10_{cis}' + 5_{trans}	5_{cis} + 11c	7.3
10_{cis}' + 5_{cis}	5_{cis} + 11b	3.4
10_{cis}' + 5_{cis}	5_{cis} + 11d	3.3
10_{cis}' + 5_{cis}	5_{cis} + 11a	1.2
10_{trans} + 6	5_{trans} + 8c	-11.0
10_{trans} + 5_{trans}	5_{trans} + 11c	-6.6
10_{trans} + 5_{cis}	5_{trans} + 11a	-12.6
10_{trans} + 5_{cis}	5_{trans} + 11b	-10.4
10_{trans} + 5_{cis}	5_{trans} + 11d	-10.6
10_{cis} + 6	5_{cis} + 8c	-9.6
10_{cis} + 5_{trans}	5_{cis} + 11c	-5.2
10_{cis} + 5_{cis}	5_{cis} + 11a	-11.2
10_{cis} + 5_{cis}	5_{cis} + 11b	-9.0
10_{cis} + 5_{cis}	5_{cis} + 11d	-9.2
5_{cis} + 8c	6 + 11a	-1.6
5_{trans} + 8c	6 + 11c	4.4
5_{cis} + 8c	6 + 11d	0.4
5_{cis} + 8c	6 + 11b	0.6
8a + 5_{trans}	6 + 11c	4.2
8a + 5_{cis}	6 + 11a	-1.8
8a + 5_{cis}	6 + 11b	0.4
8a + 5_{cis}	6 + 11d	0.2
8b + 5_{trans}	6 + 11c	3.6
8b + 5_{cis}	6 + 11a	-2.4
8b + 5_{cis}	6 + 11b	-0.2
8b + 5_{cis}	6 + 11d	-0.4

Characterization data for unreported sulfone starting materials (6)

4-Bromobenzyl 2-phenylethynyl sulfone was obtained as a white solid. Yield: 44%. Mp: 157 – 158 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.55 (m, 5H, Ar H), 7.50 (m, 2H, Ar H), 7.38 (m, 2H, Ar H), 4.48 (s, 2H, CH₂). ¹³C NMR (100.6 MHz, CDCl₃): δ 132.87, 132.80, 132.18, 131.95, 128.88, 126.23, 124.06, 117.28, 94.49, 82.37, 63.89. IR (cm⁻¹, neat): 2988, 2181, 1487, 1328, 1149, 1126, 887, 750. Analysis calculated for C₁₅H₁₁BrO₂S; C, 53.74; H, 3.31; found C, 53.60; H, 3.50.

4-Methylbenzyl 2-phenylethynyl sulfone was obtained as a white solid. Yield: 90%. Mp: 75-76 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.50 (m, 3H, Ar H), 7.41 (m, 4H, Ar H), 7.25 (m, 2H, Ar H), 4.49 (s, 2H, CH₂), 2.41 (s, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ 132.78, 131.73, 131.21, 129.42, 128.87, 128.62, 127.42, 117.46, 94.16, 82.54, 64.62, 21.21; IR (cm⁻¹, neat): 3061, 2979, 2921, 2183, 1512, 1488, 1443, 1199, 1149, 1126, 759. Analysis calculated for C₁₆H₁₄O₂S; C, 71.08; H, 5.22; found C, 71.23; H, 5.40.

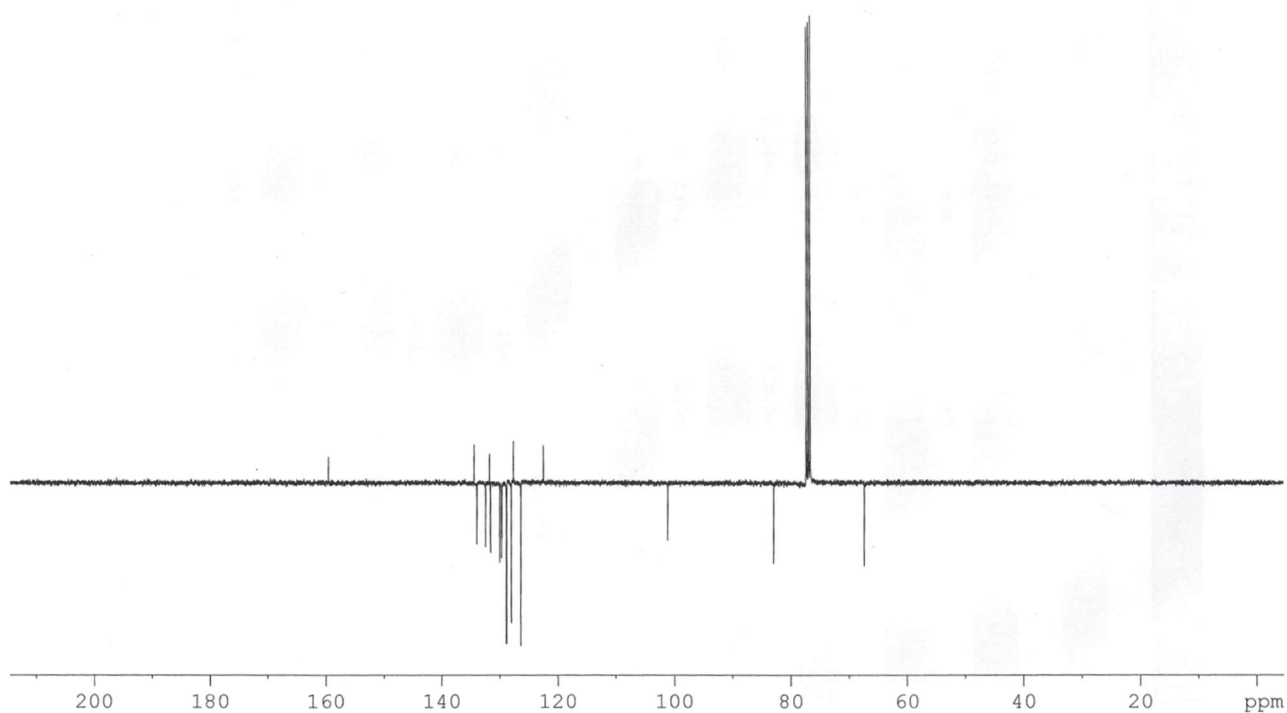
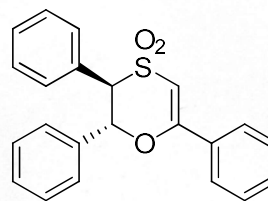
4-Methoxybenzyl 2-phenylethynyl sulfone was obtained as a white solid. Yield: 65%. Mp: 74 – 75 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.51 (m, 3H, Ar H), 7.43 (m, 4H, Ar H), 6.97 (m, 2H, Ar H), 4.48 (s, 2H, CH₂), 3.85 (s, 3H, CH₃). ¹³C NMR (100.6 MHz, CDCl₃): δ 160.54, 132.82, 132.53, 131.72, 128.79, 118.96, 117.60, 114.37, 94.04, 82.67, 64.00, 55.38. IR (cm⁻¹, neat): 3001, 2967, 2838, 2182, 1610, 1328, 1305, 1253, 1127. Analysis calculated for C₁₆H₁₄O₃S; C, 67.11; H, 4.93; found C, 66.89; H, 5.24.

3-Chlorobenzyl 2-phenylethynyl sulfone was obtained as a white solid. Yield: 78%. Mp: 84 – 85 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.51 (m, 4H, Ar H), 7.46 (m, 5H, Ar H), 4.49 (s, 2H, CH₂). ¹³C NMR (100.6 MHz, CDCl₃): δ 134.73, 132.88, 131.94, 131.28, 130.20, 129.71, 129.47, 129.18, 128.86, 117.24, 94.72, 82.27, 63.95. IR (cm⁻¹, neat): 3064, 2983, 2924, 2182, 1330, 1256, 1151, 1127. ESI HRMS, calculated for [C₁₅H₁₁³⁵ClO₂S+NH₄]⁺: 308.0507; found: 308.0496.

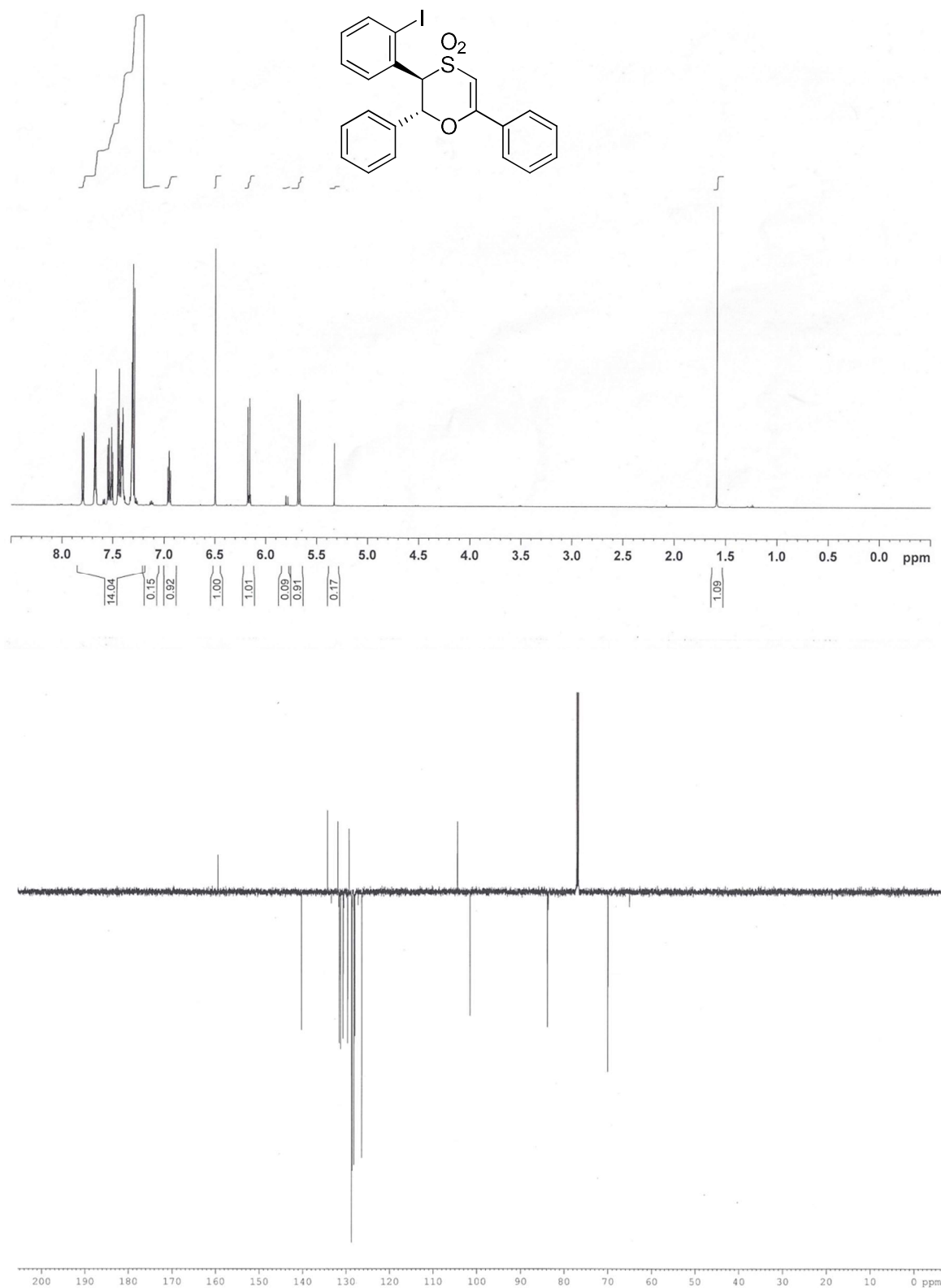
4-Nitrobenzyl 2-phenylethynyl sulfone (82h) was obtained as a white solid. Yield: 64%. Mp: 169 – 170 °C. ¹H NMR (400 MHz, CDCl₃): δ 7.53 (m, 9H, ArH), 4.49 (s, 2H, CH₂). ¹³C NMR (100.6 MHz, CDCl₃): δ 134.15, 132.91, 131.94, 130.49, 129.93, 128.86, 122.75, 117.22, 94.78, 82.24, 63.89. IR (cm⁻¹, neat): 3077, 3061, 2932, 2181, 1522, 1490, 1348, 1332, 1150, 1127. Analysis calculated for C₁₅H₁₁NO₄S; C, 59.79; H, 3.68; found C, 59.55; H, 3.71.

NMR Spectra for Compounds 5 and 7.

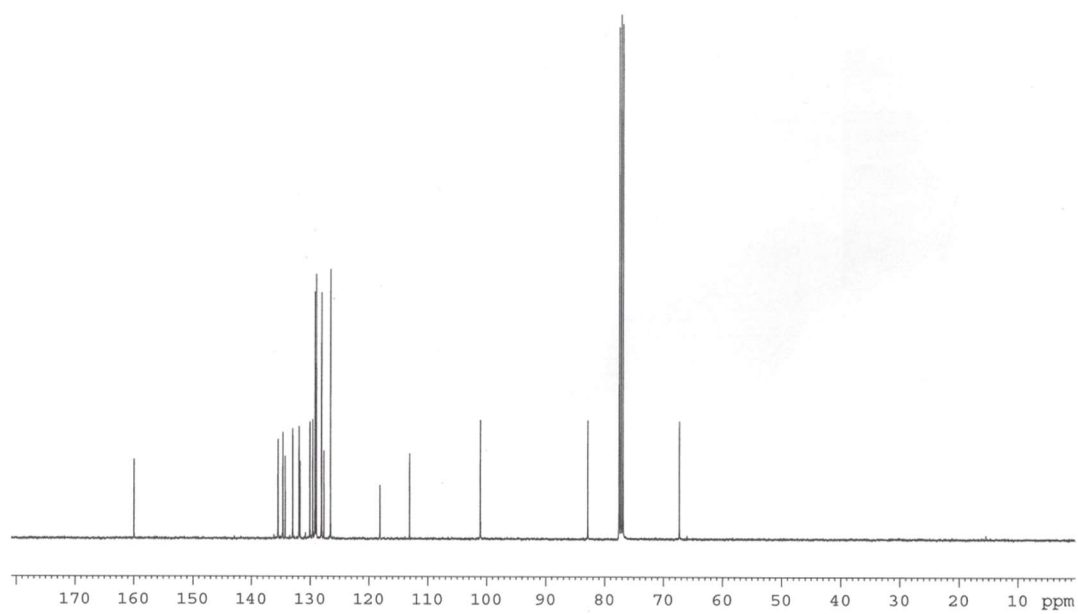
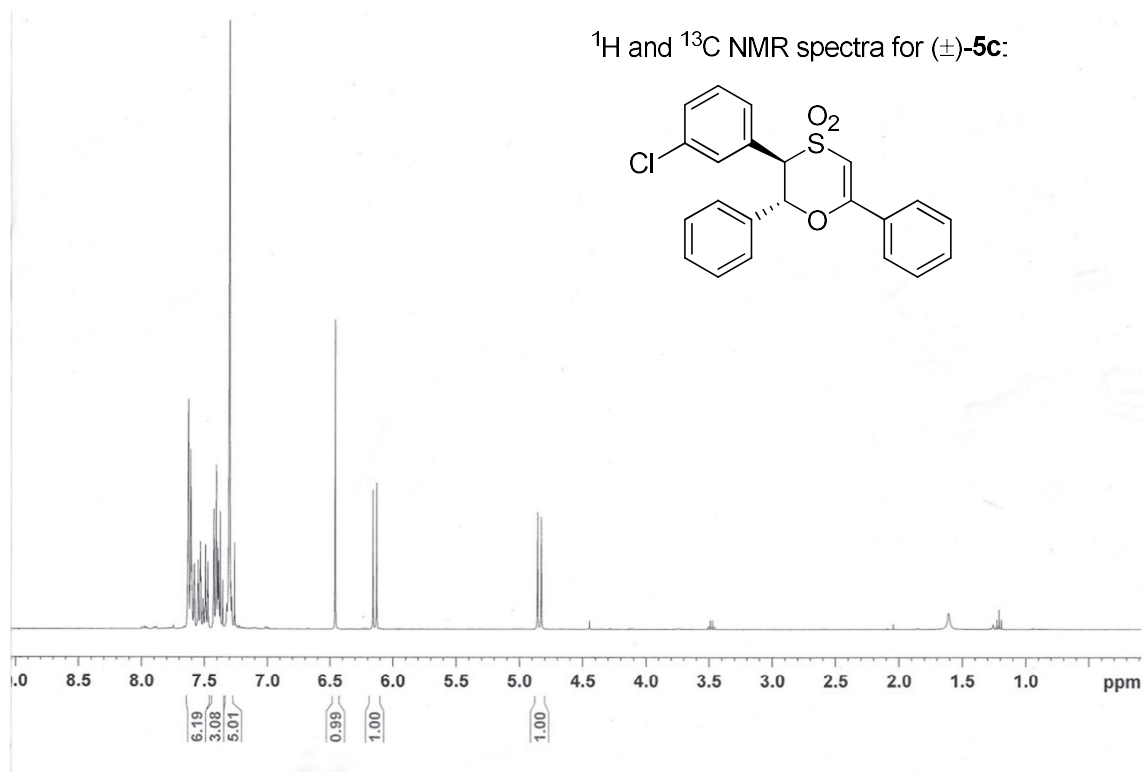
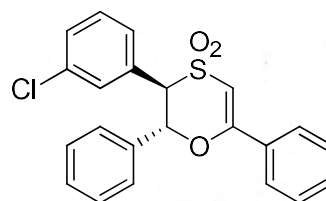
NMR spectra for (±)-**5a**:



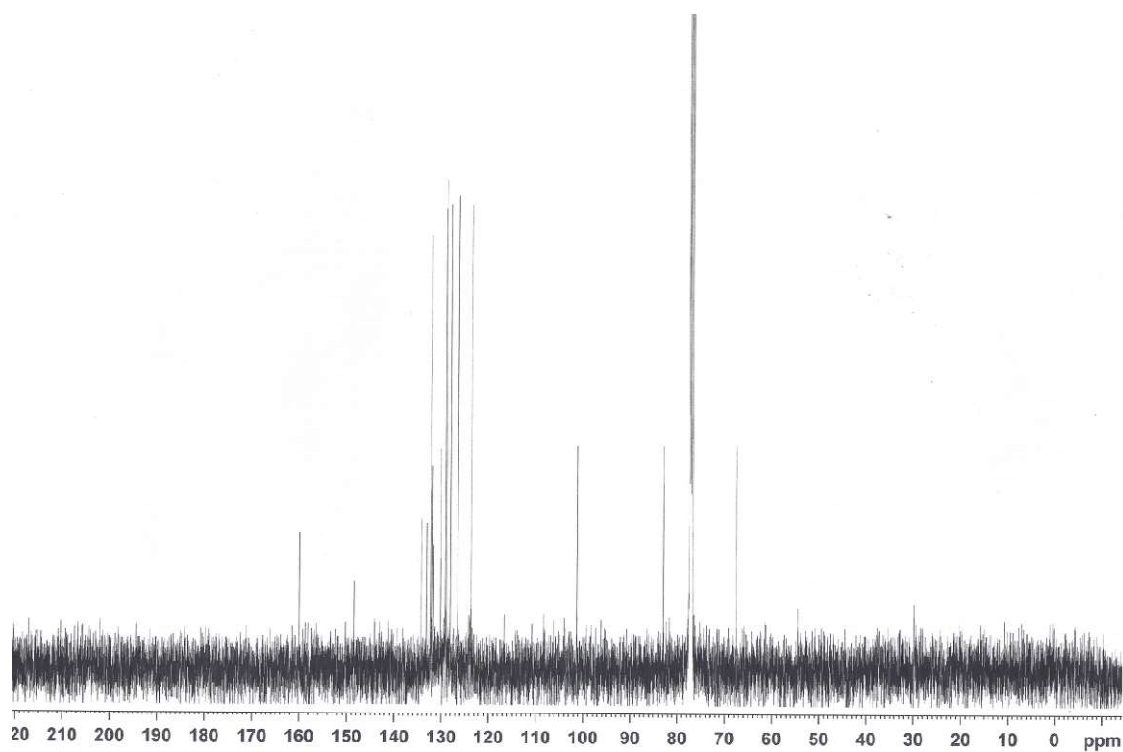
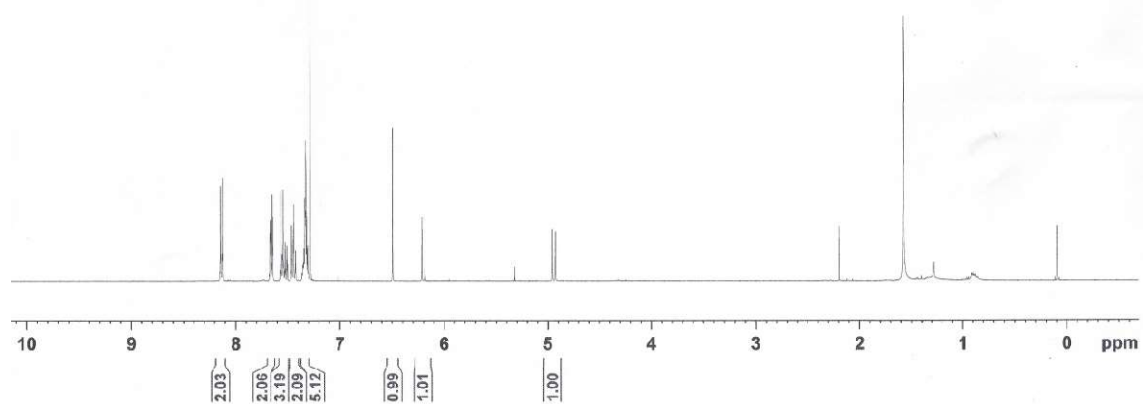
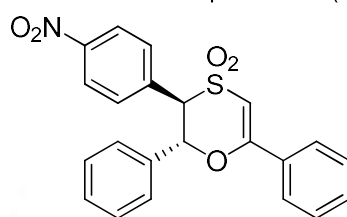
^1H and ^{13}C NMR spectra for ($\pm$)-**5b**:



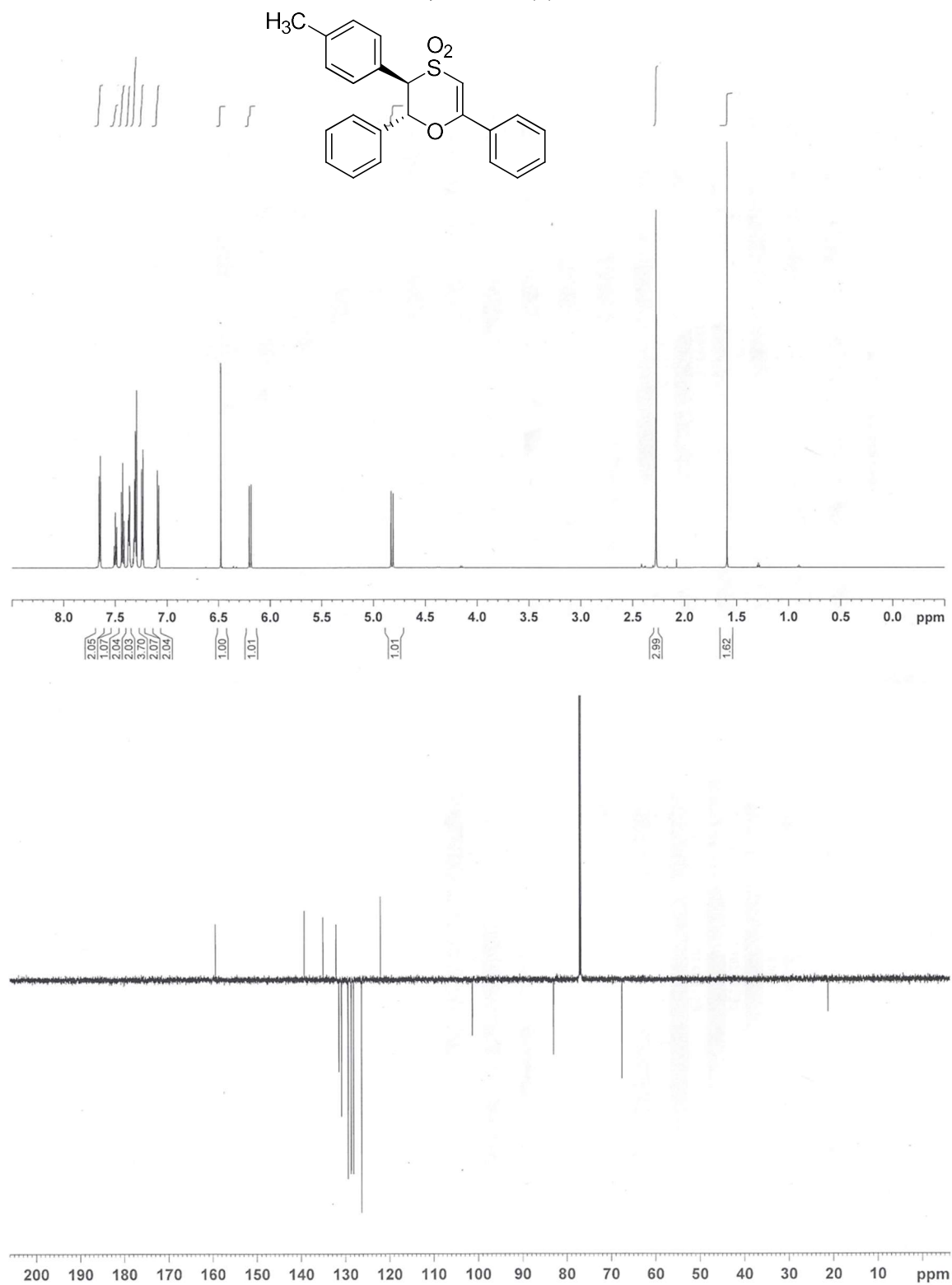
^1H and ^{13}C NMR spectra for ($\pm$)-**5c**:



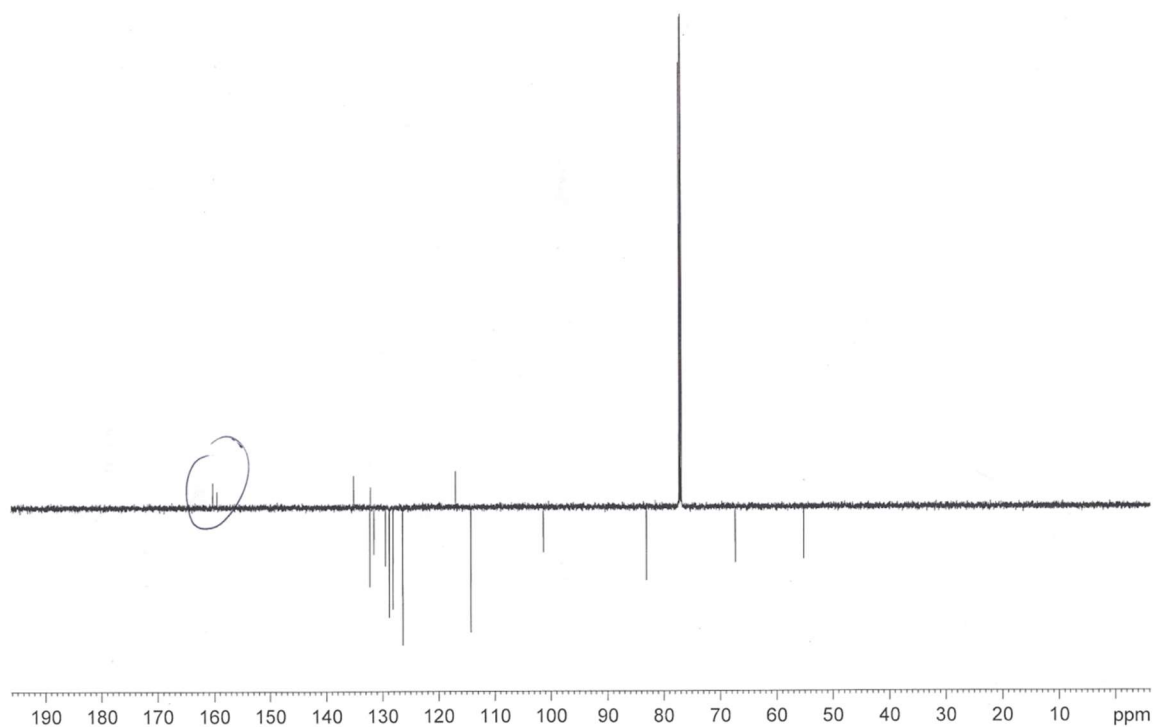
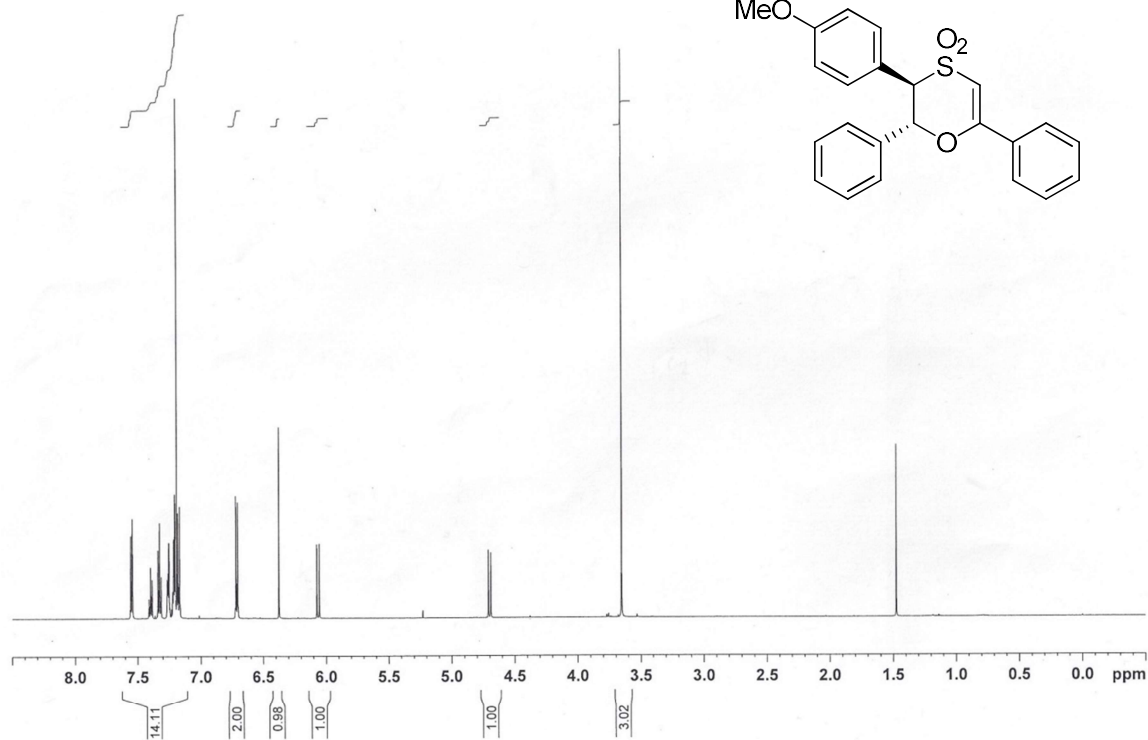
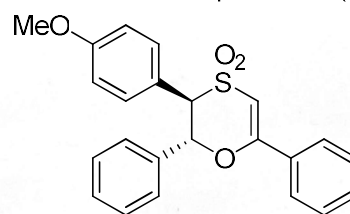
^1H and ^{13}C NMR spectra for ($\pm$)-**5d**:



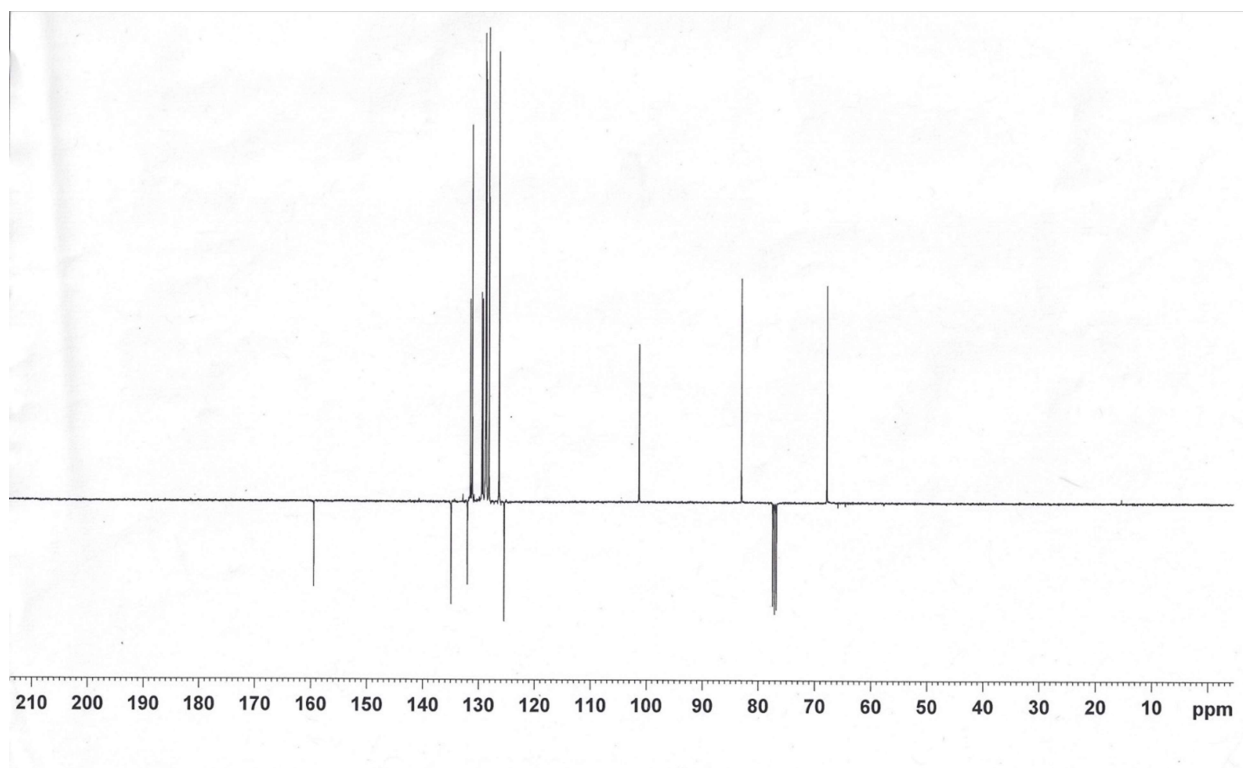
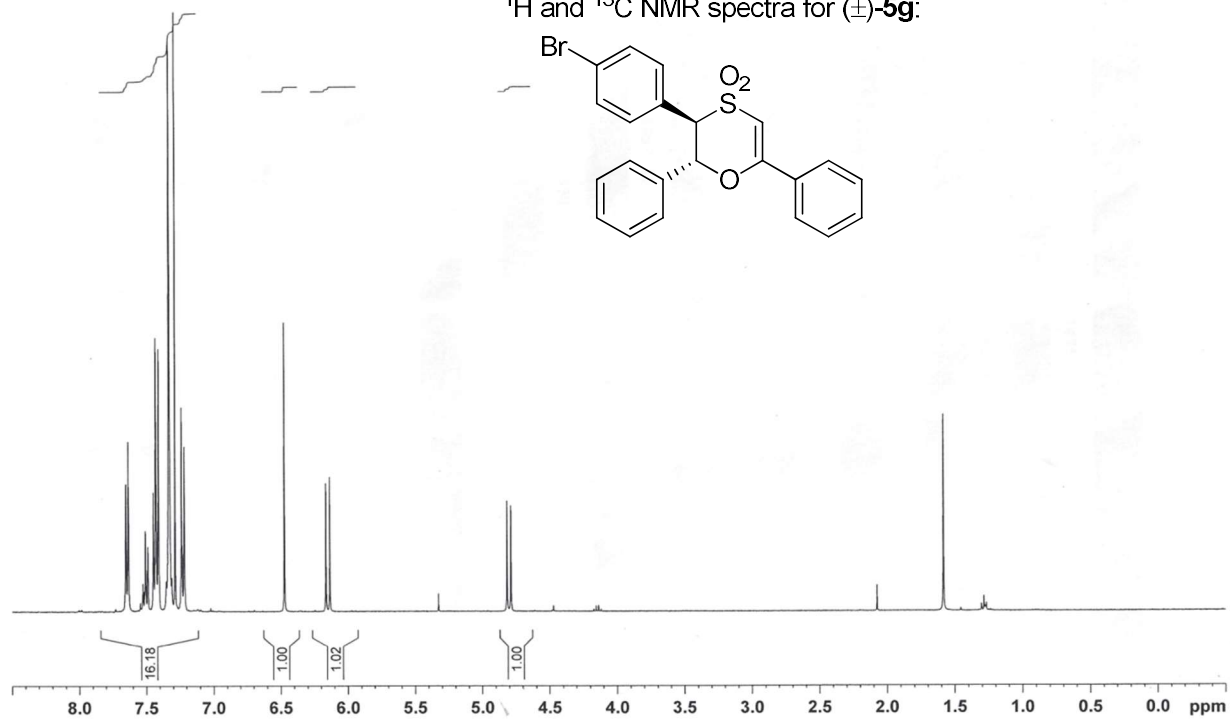
^1H and ^{13}C NMR spectra for ($\pm$)-**5e**:



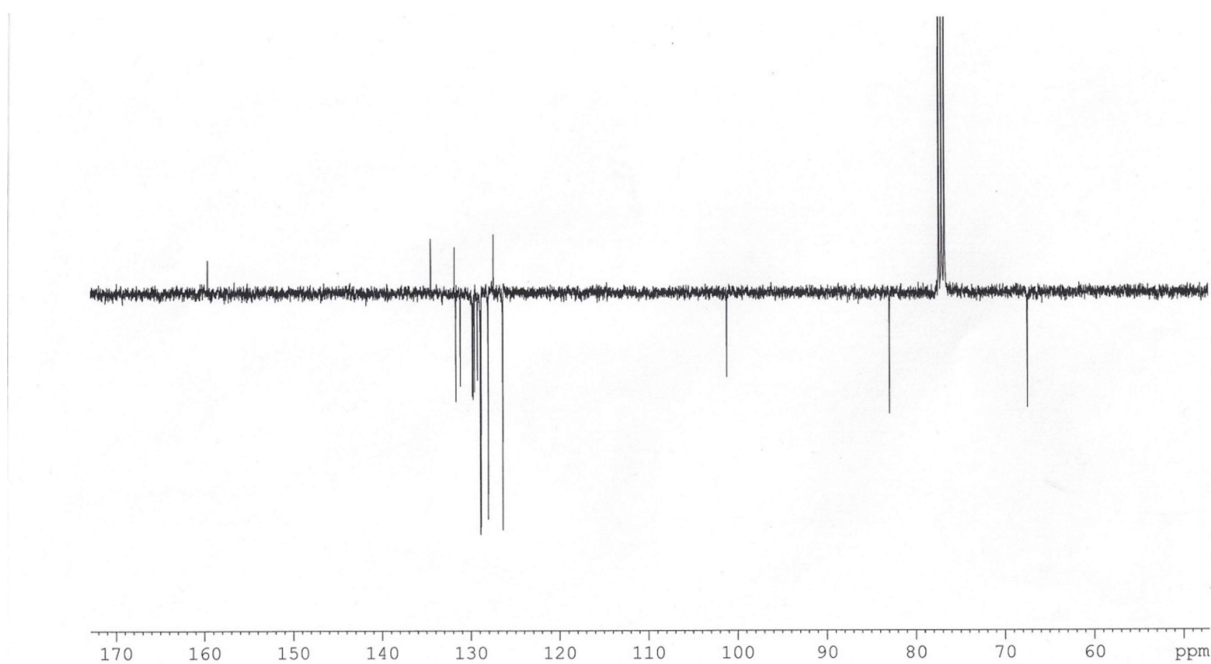
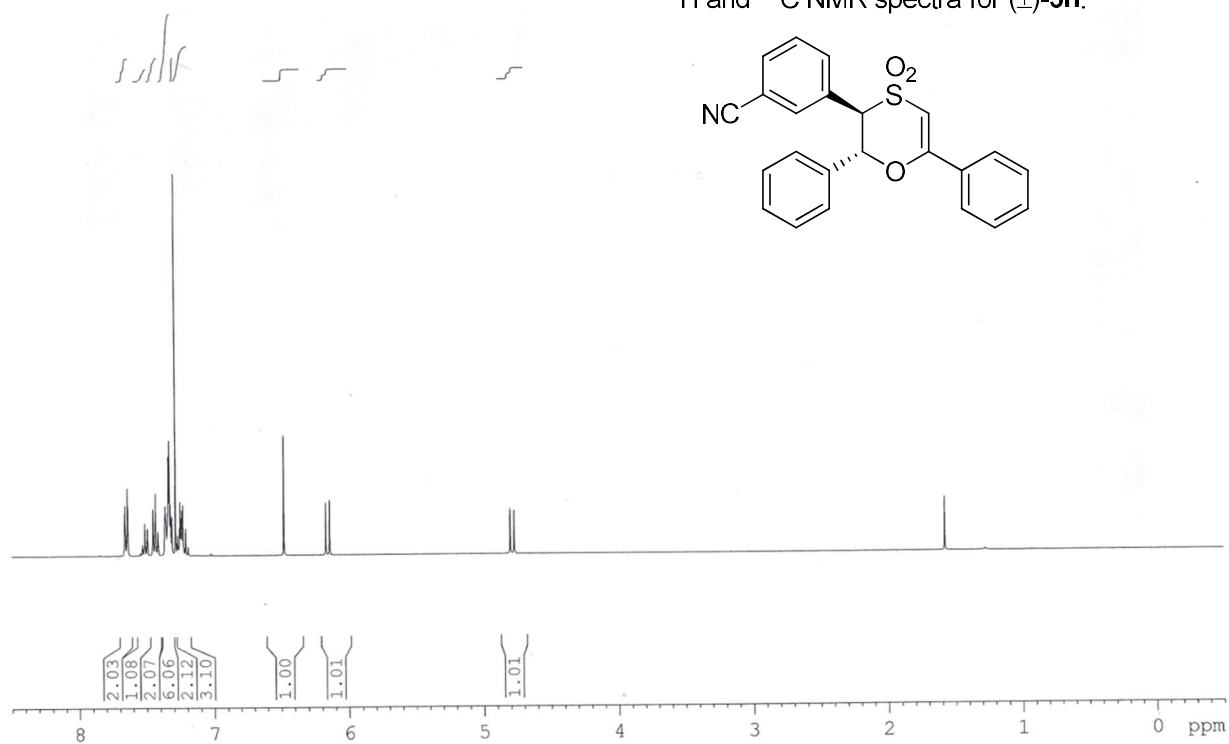
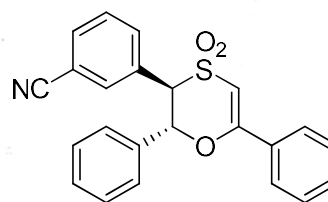
^1H and ^{13}C NMR spectra for ($\pm$)-**5f**:



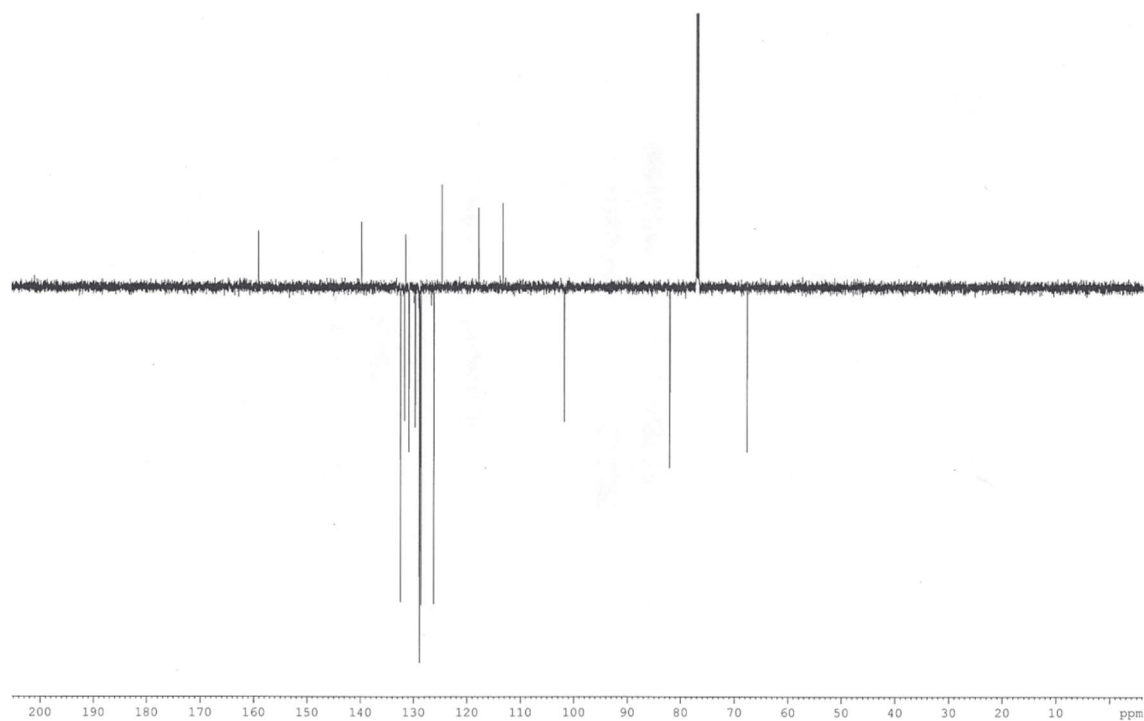
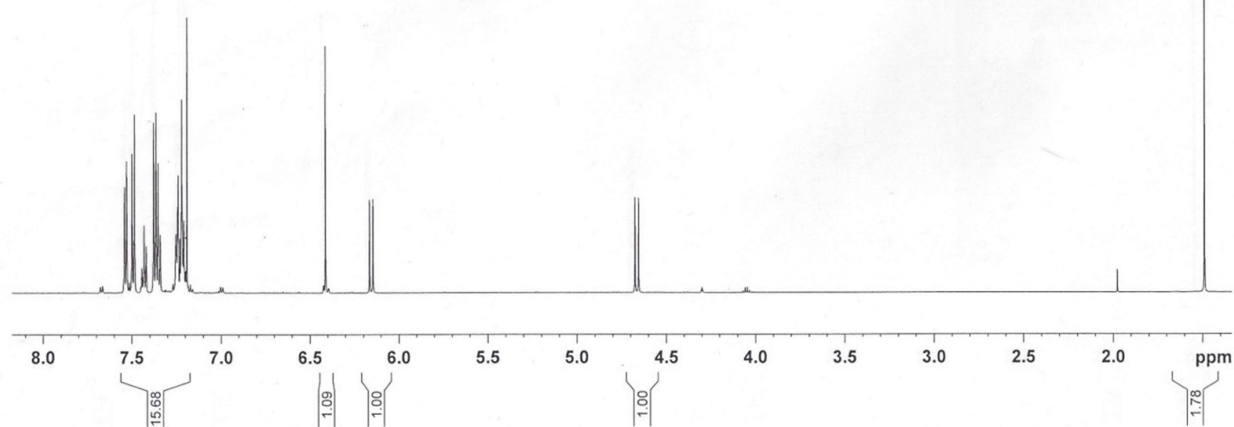
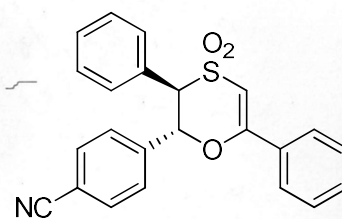
^1H and ^{13}C NMR spectra for ($\pm$)-**5g**:



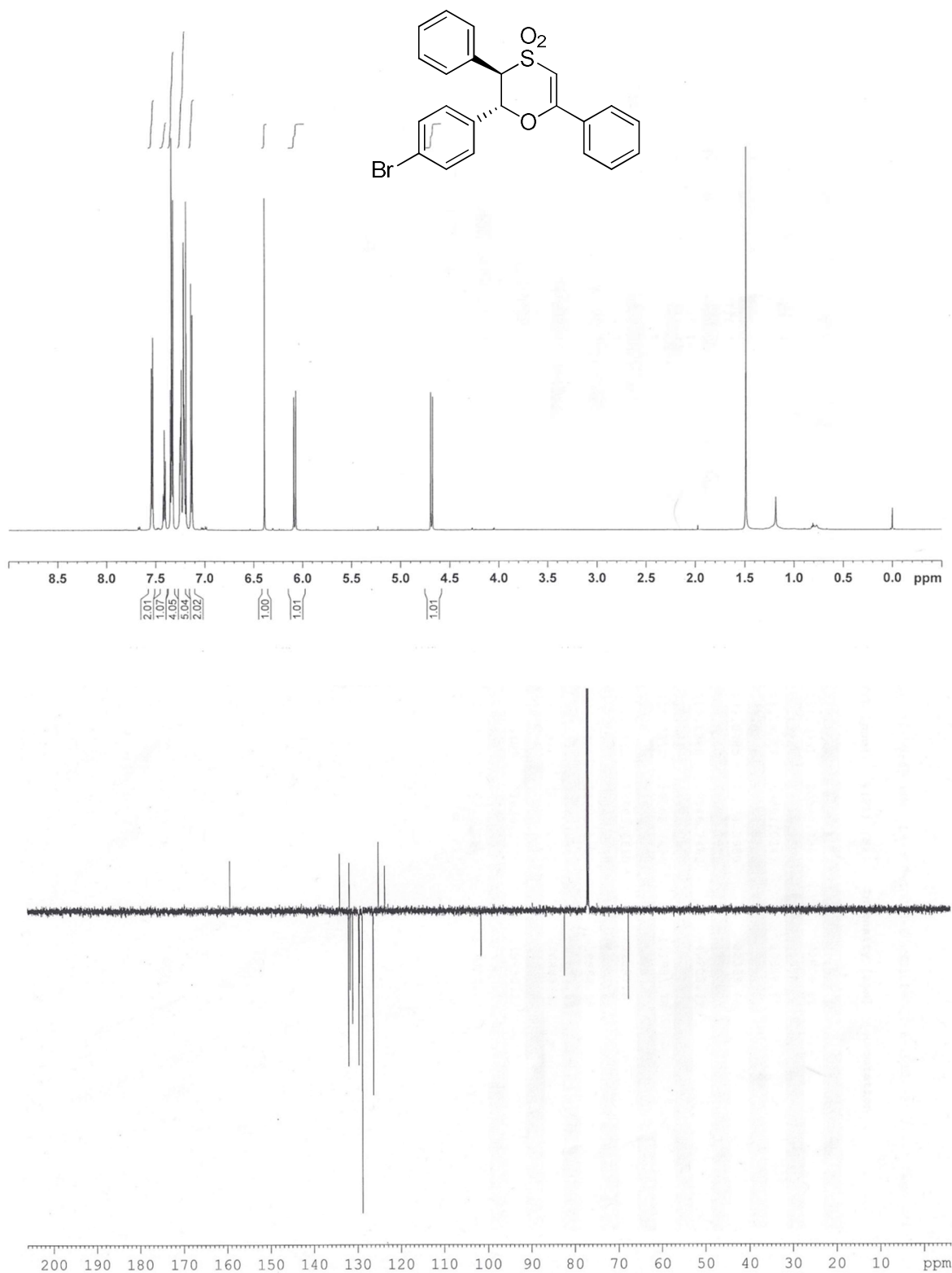
^1H and ^{13}C NMR spectra for ($\pm$)-**5h**:



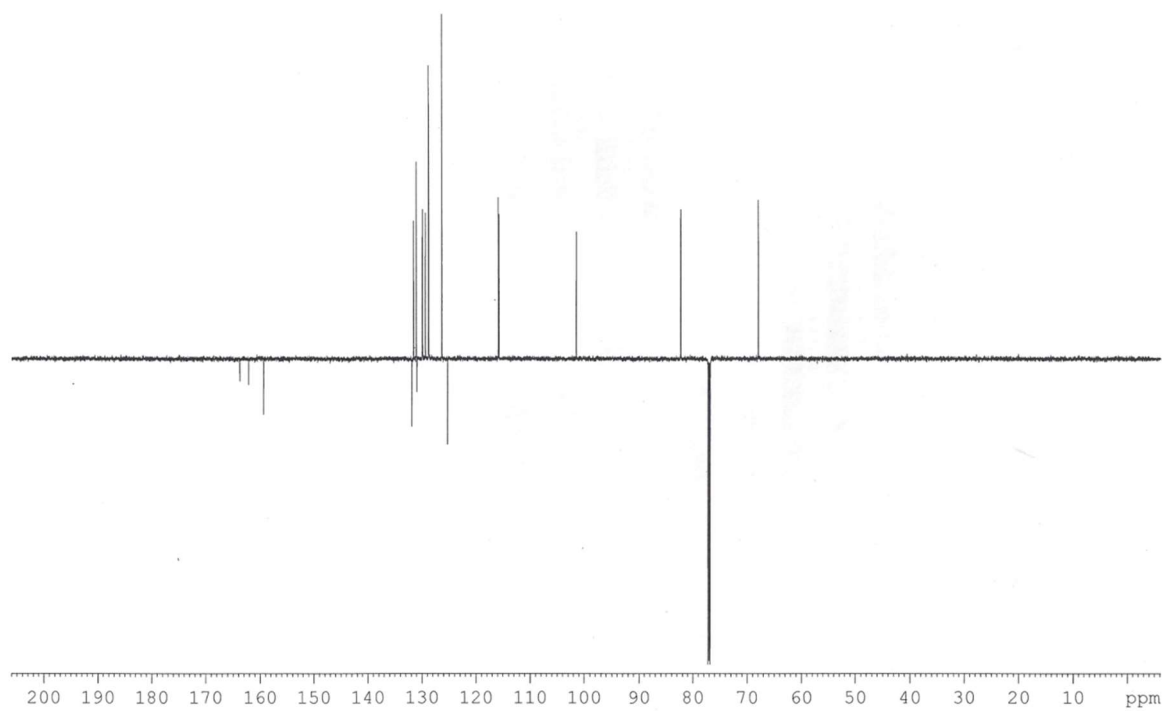
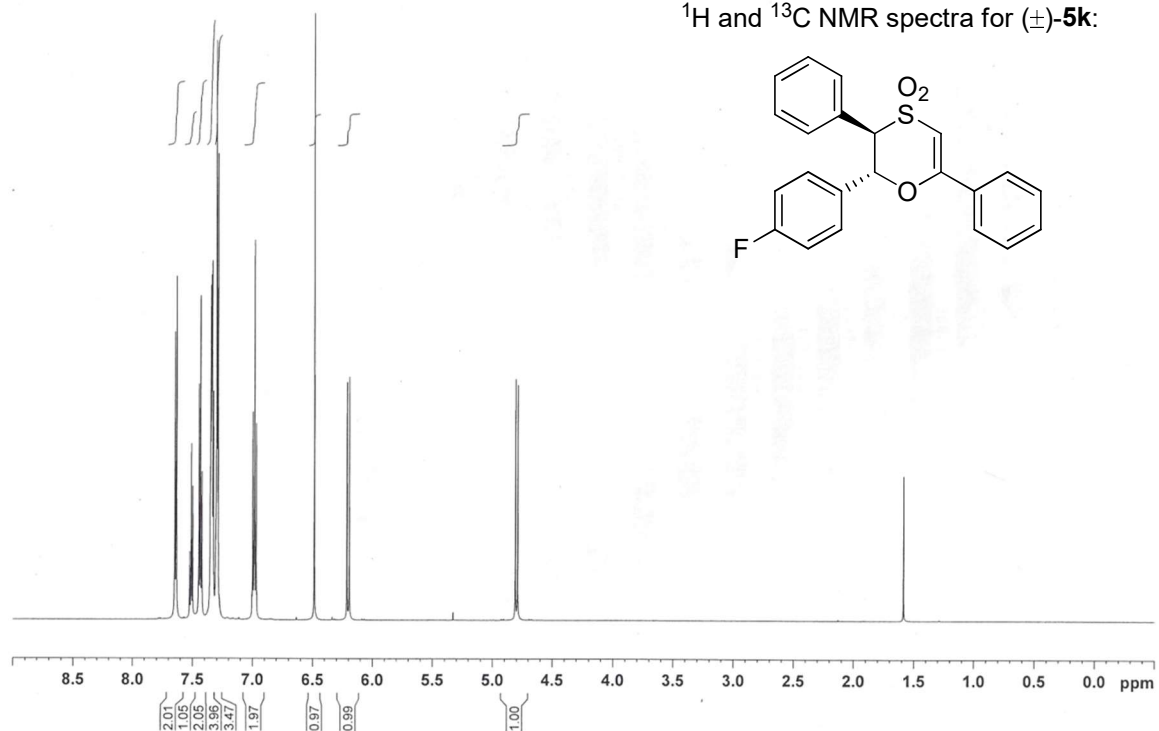
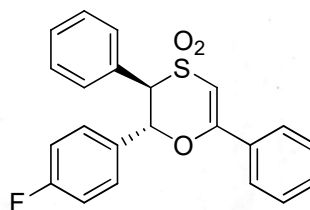
^1H and ^{13}C NMR spectra for ($\pm$)-**5i**:



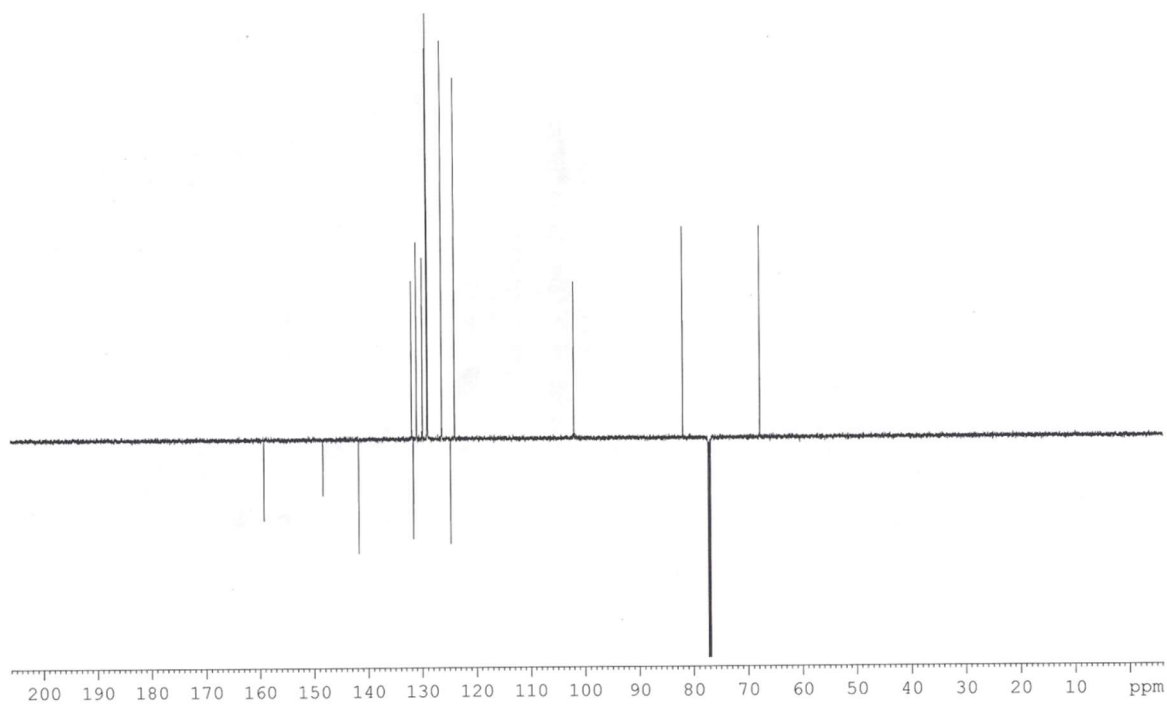
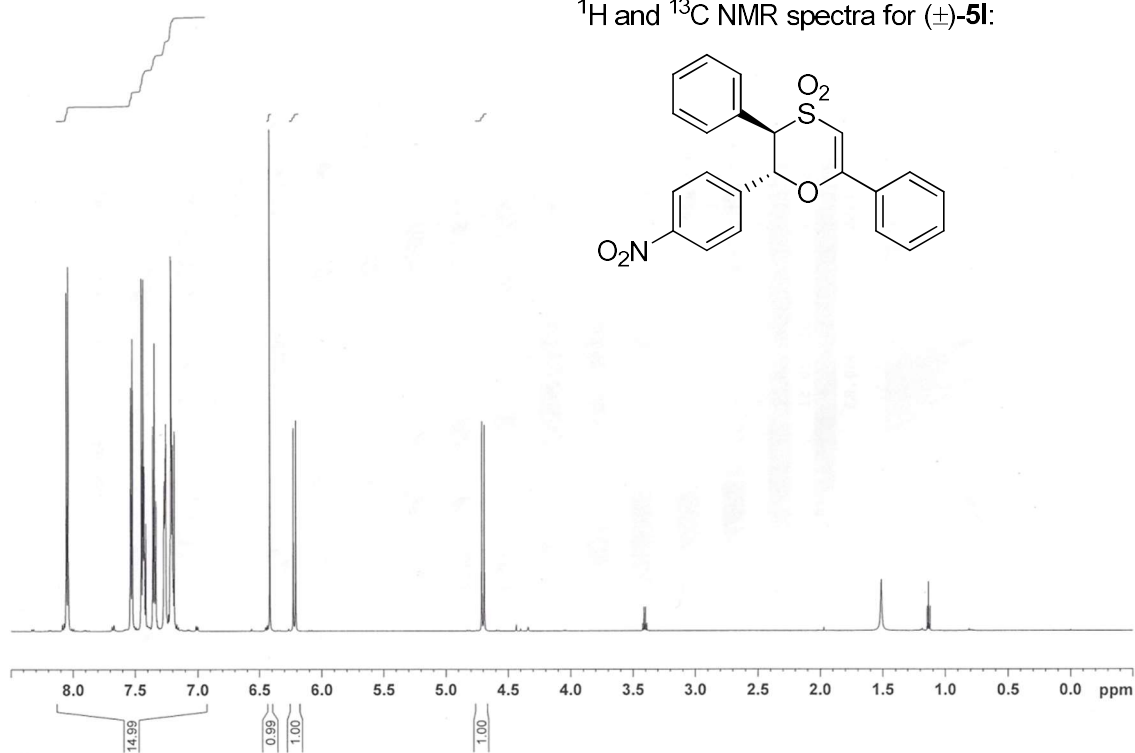
^1H and ^{13}C NMR spectra for ($\pm$)-**5j**:



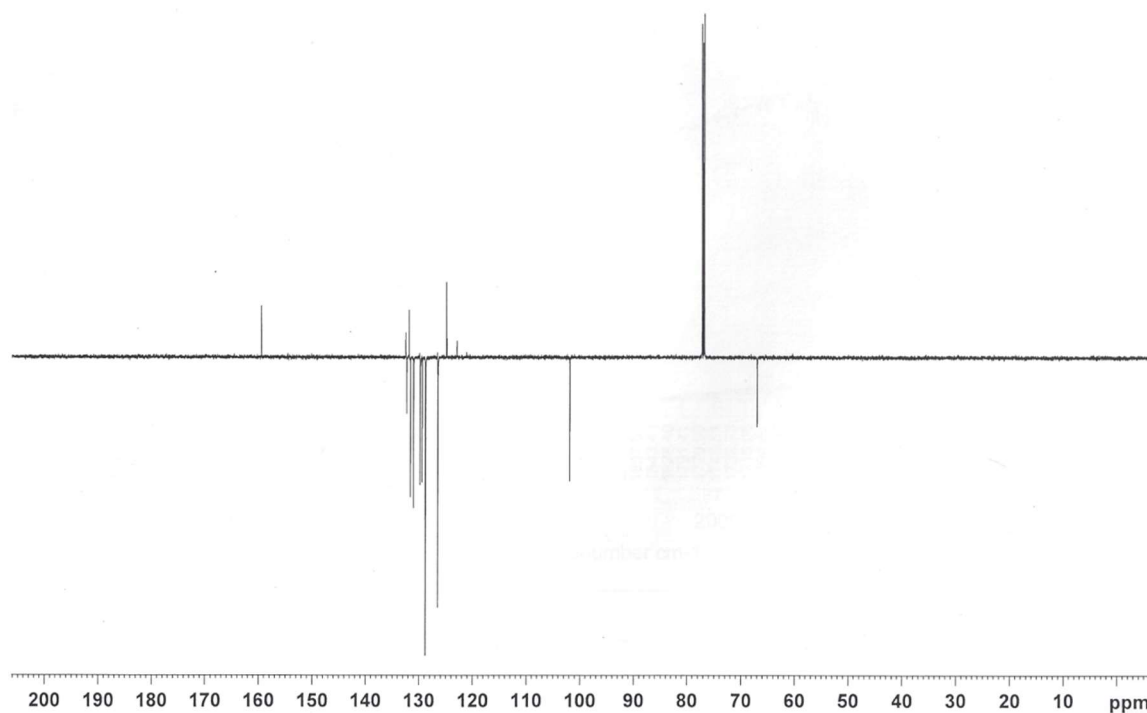
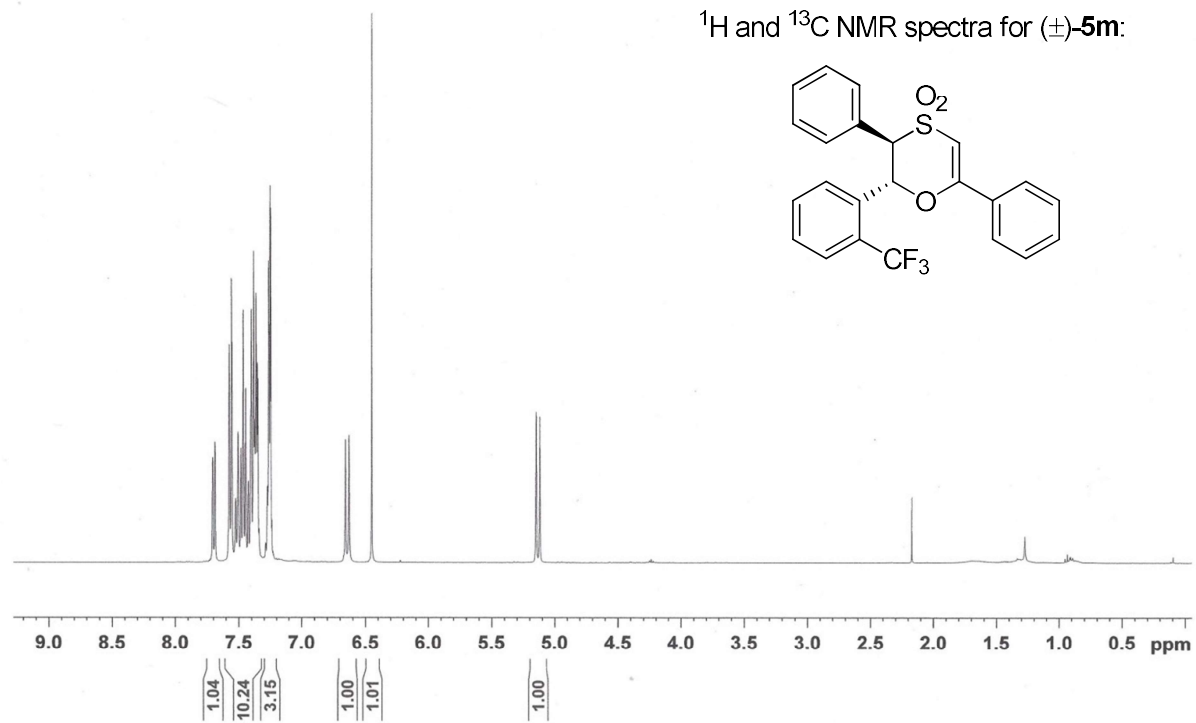
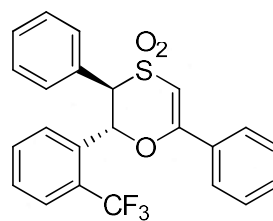
^1H and ^{13}C NMR spectra for ($\pm$)-**5k**:

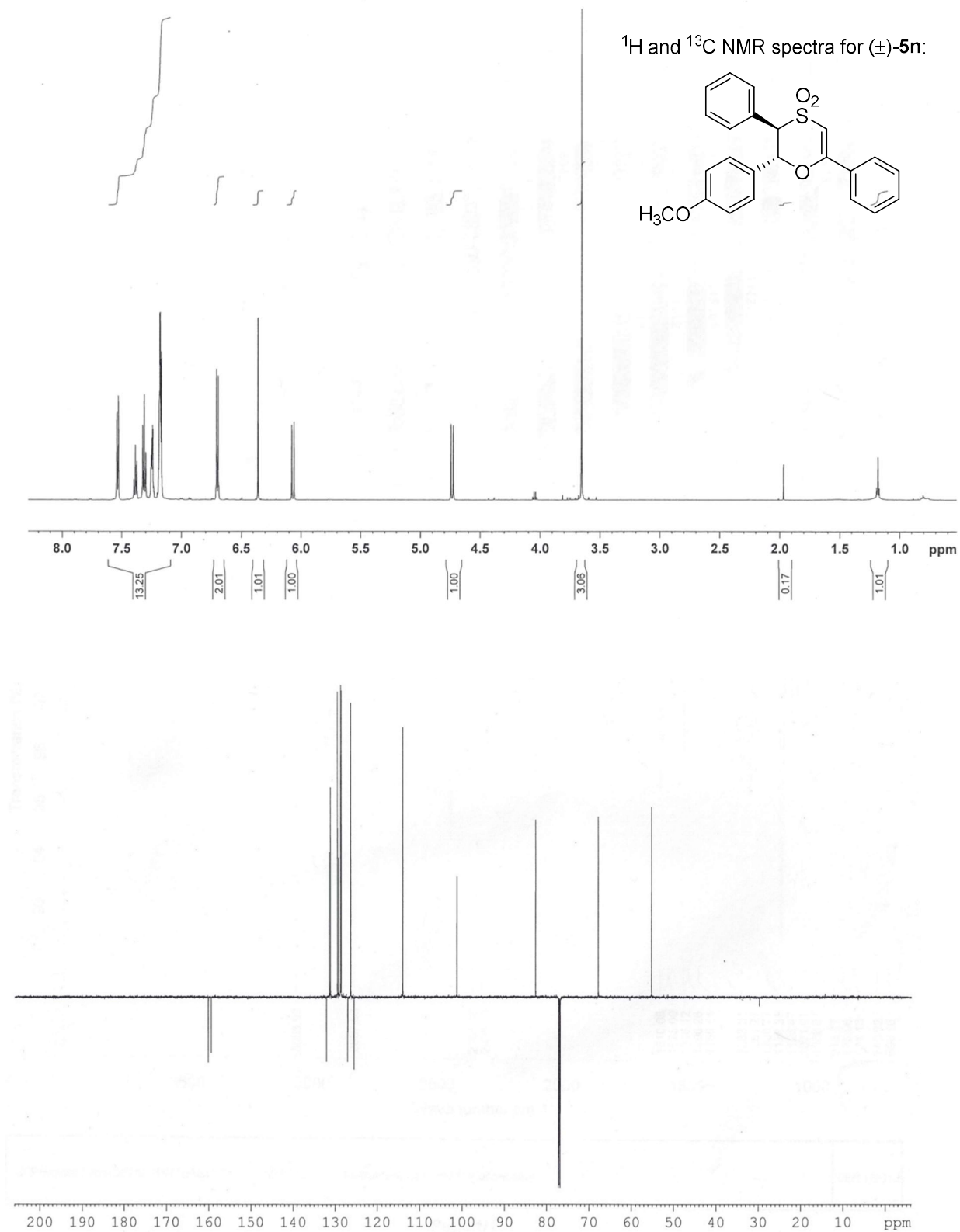


^1H and ^{13}C NMR spectra for ($\pm$)-**5l**:

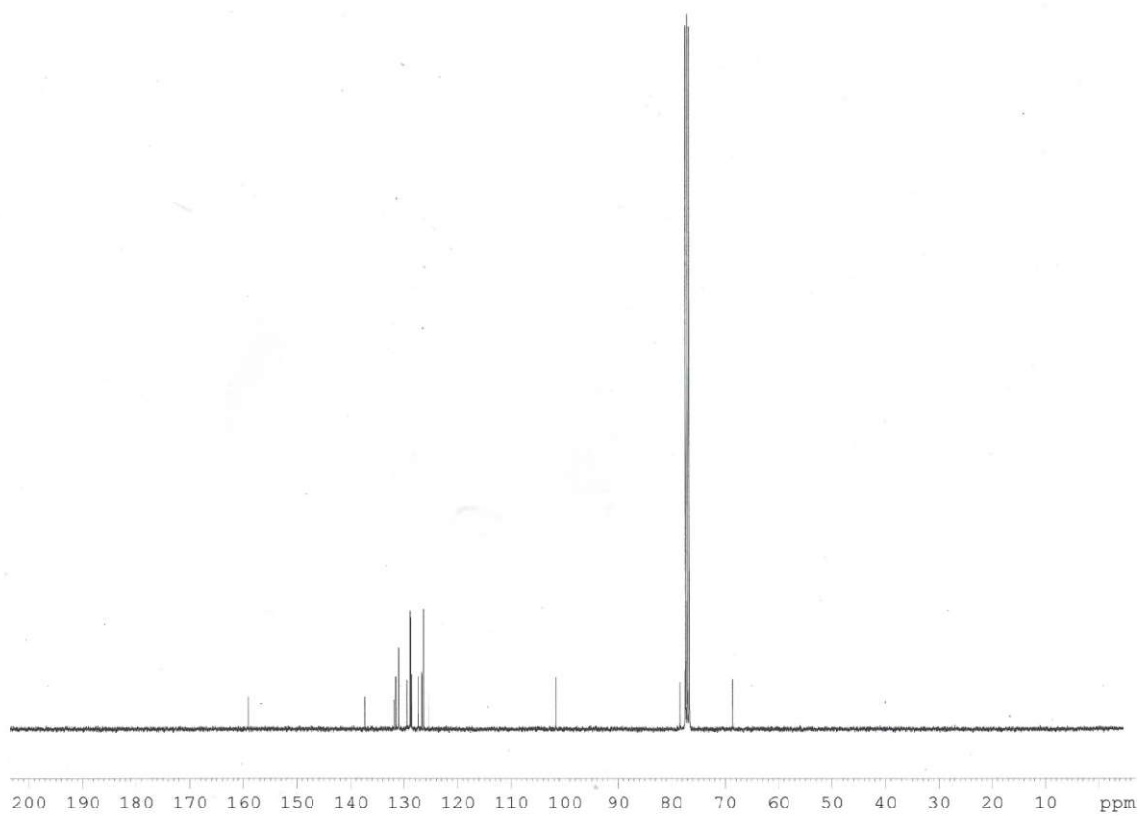
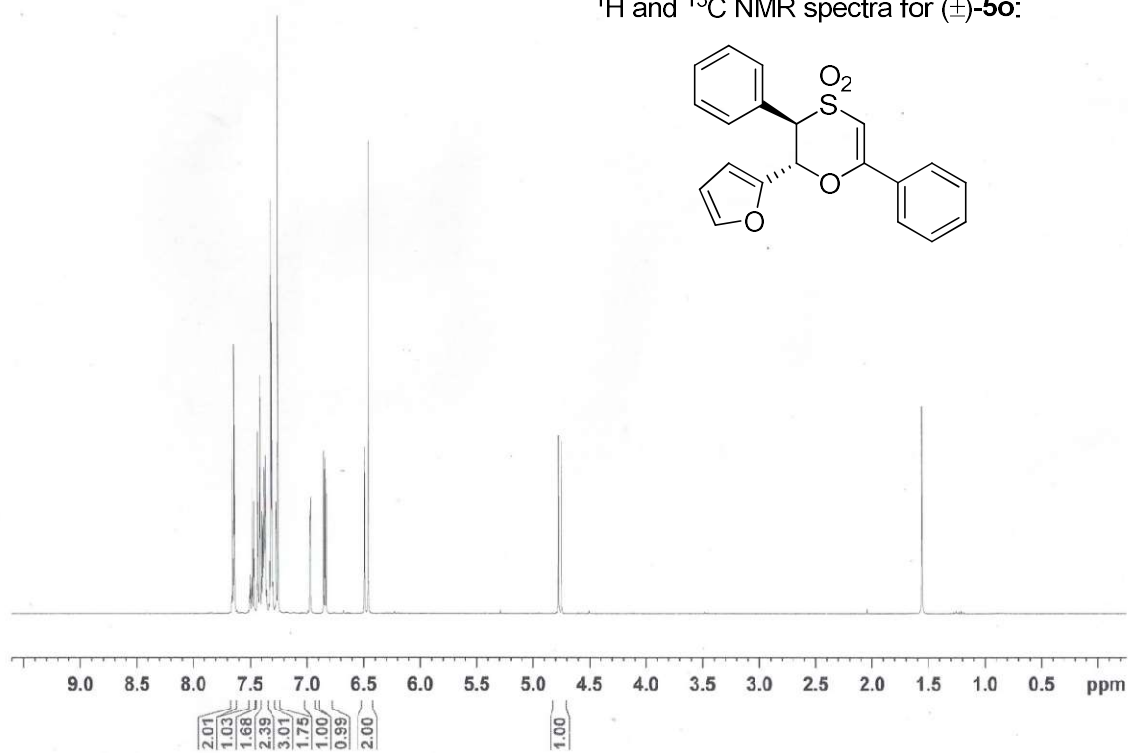
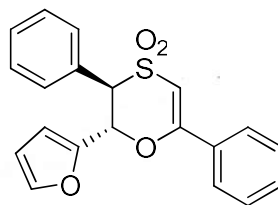


^1H and ^{13}C NMR spectra for ($\pm$)-**5m**:

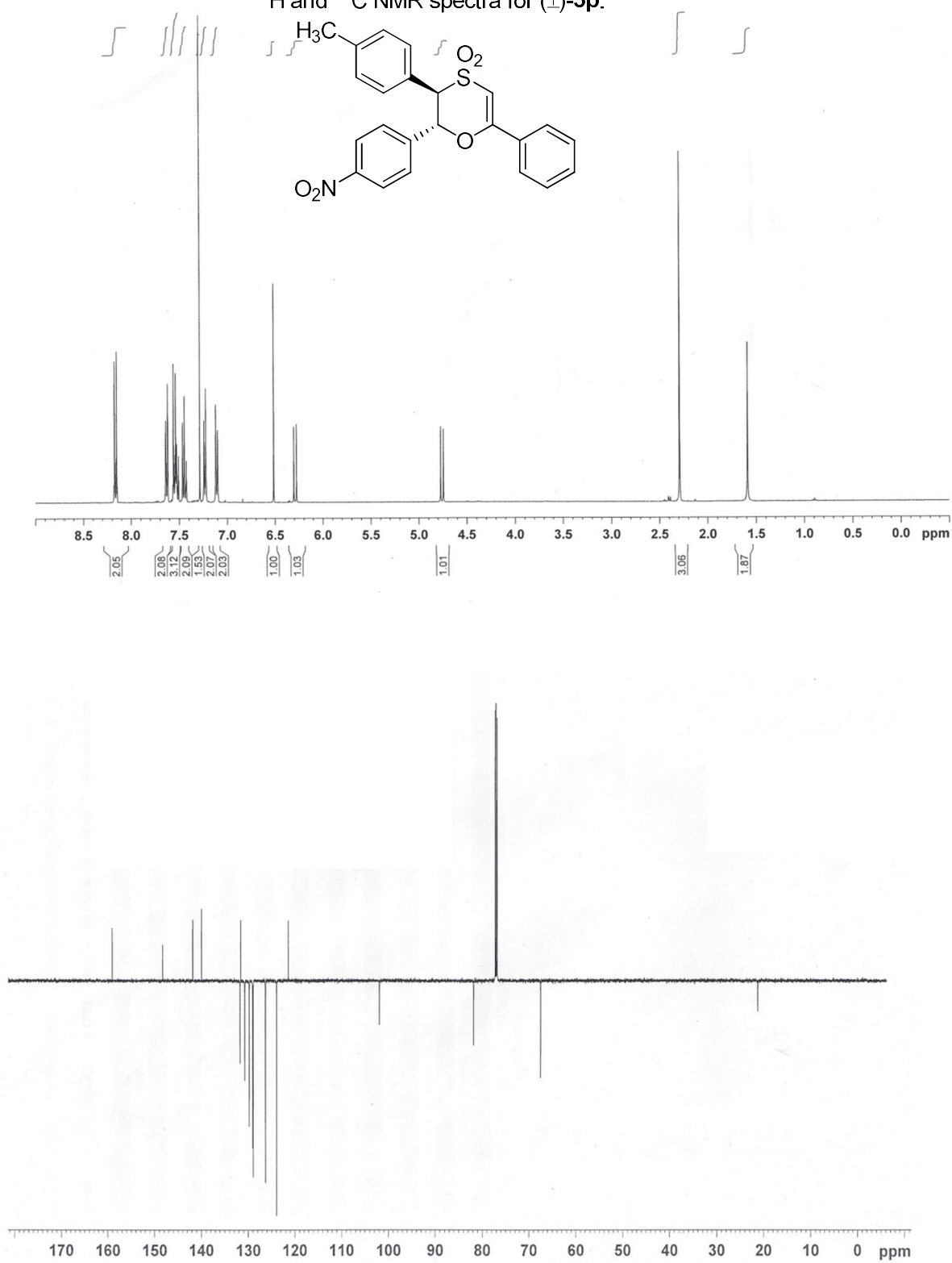




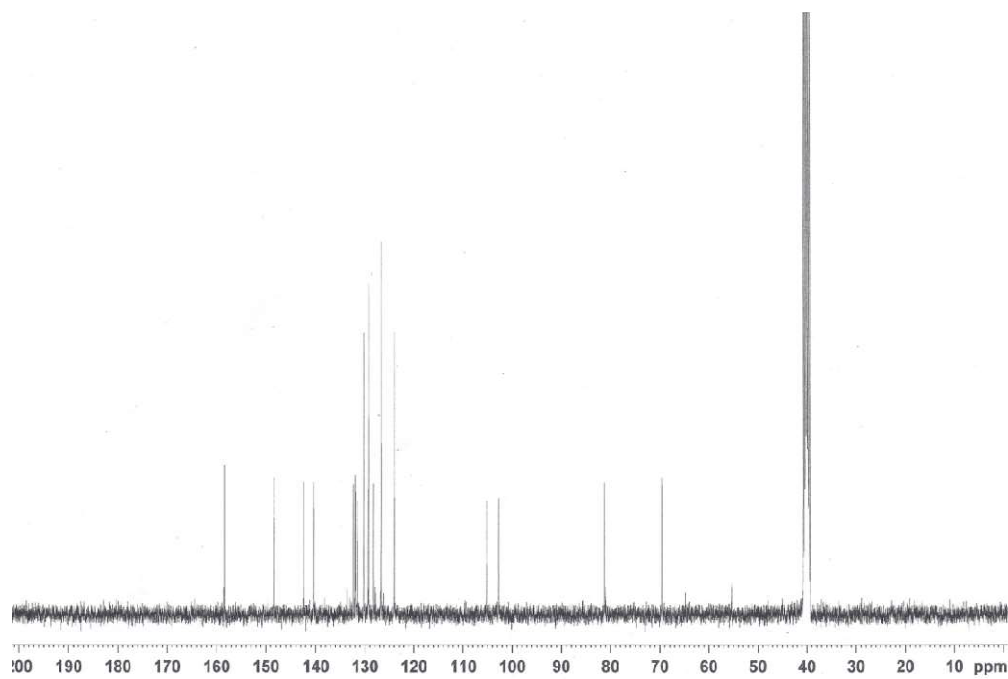
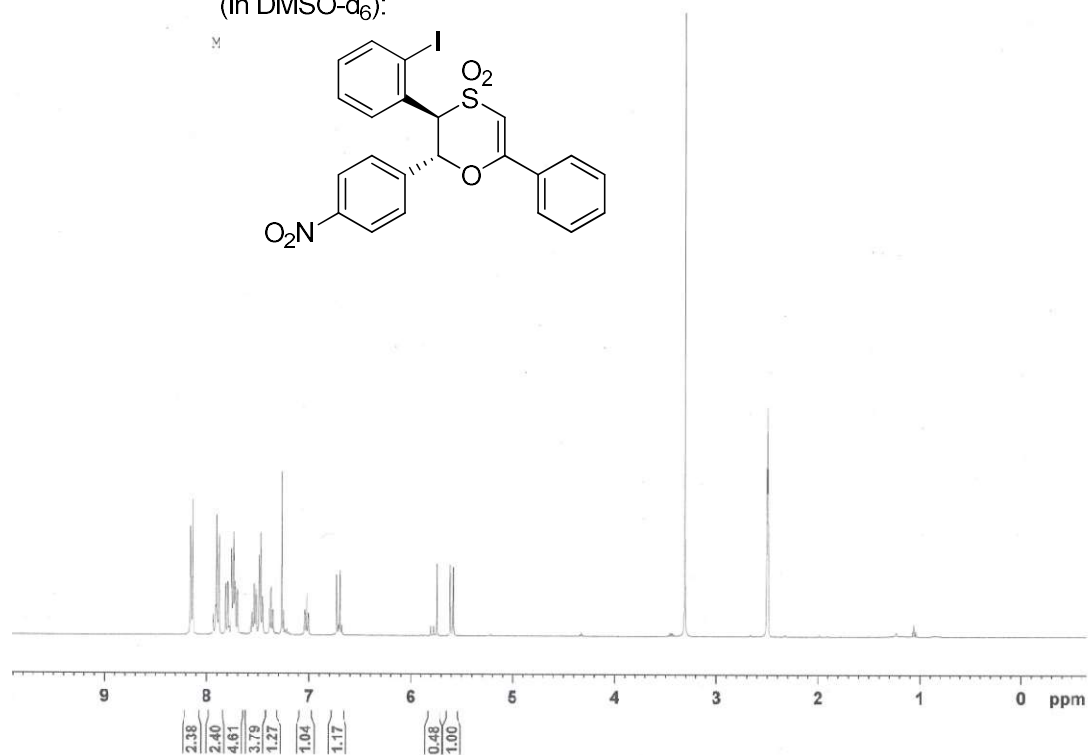
^1H and ^{13}C NMR spectra for ($\pm$)-**5o**:



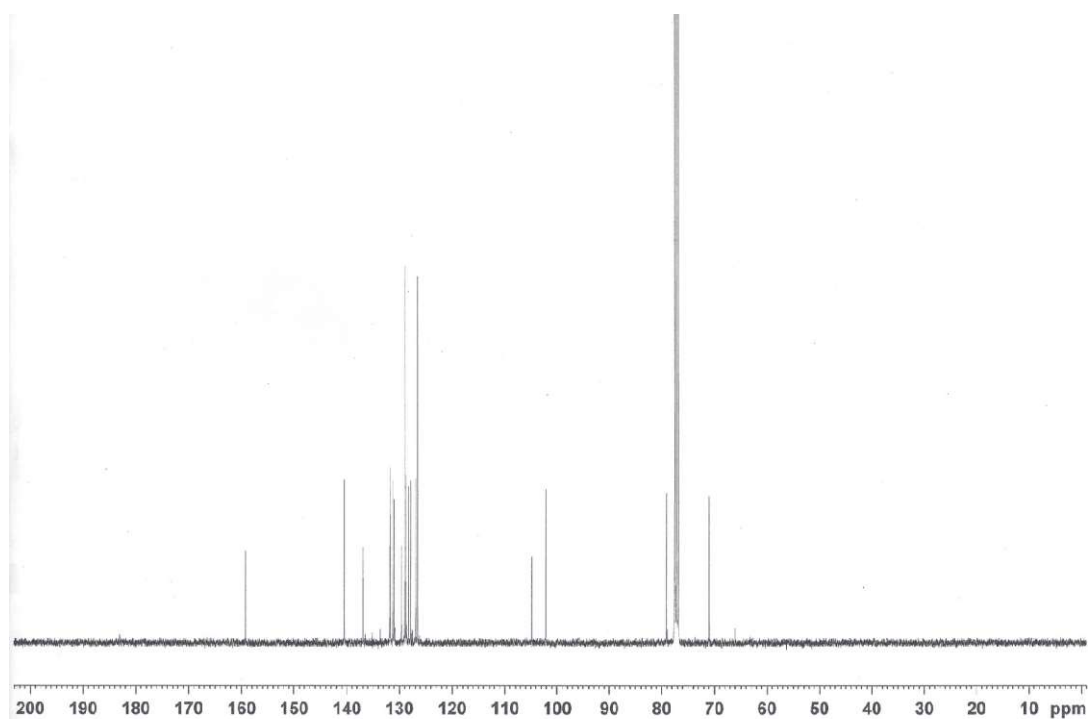
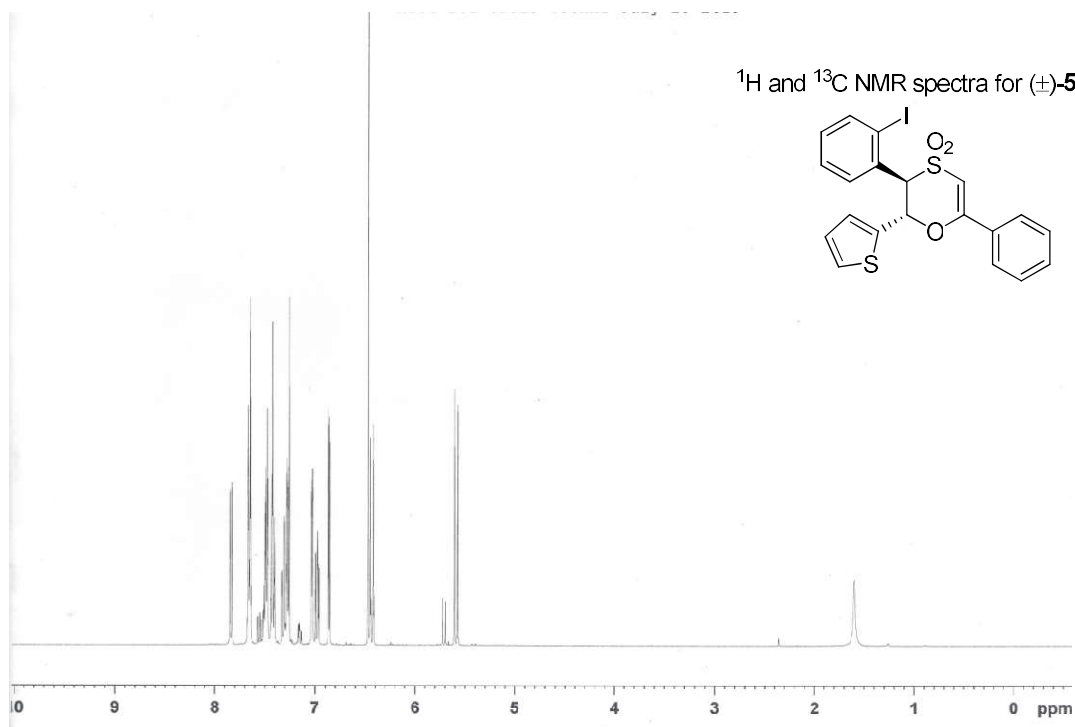
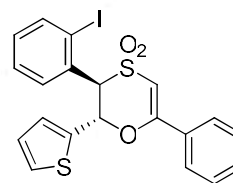
^1H and ^{13}C NMR spectra for ($\pm$)-**5p**:



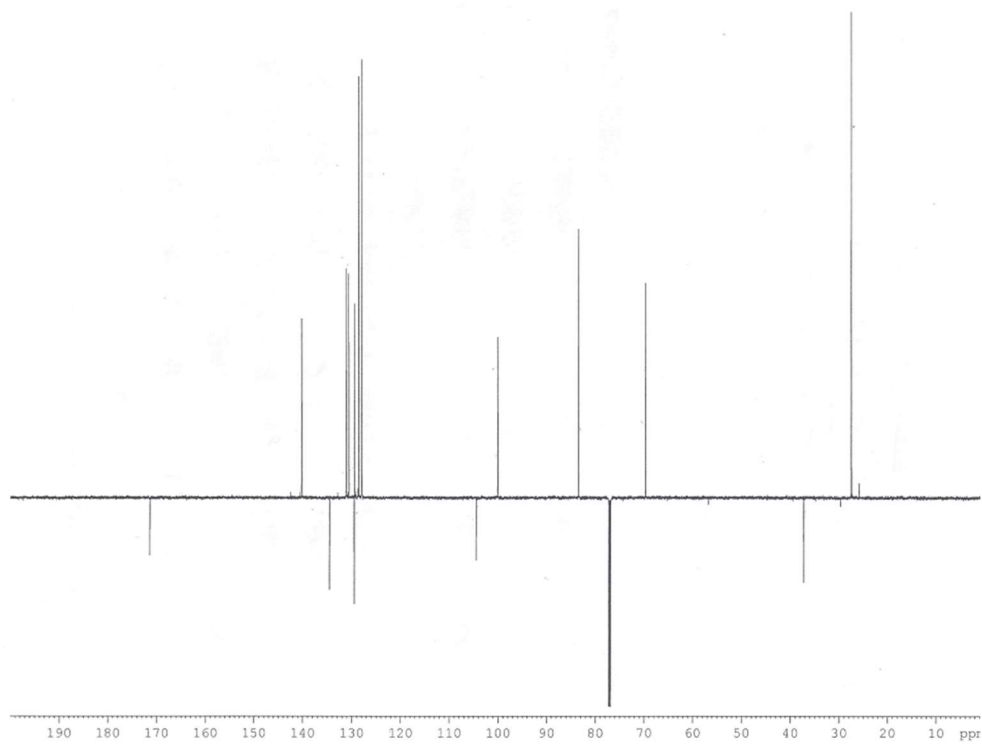
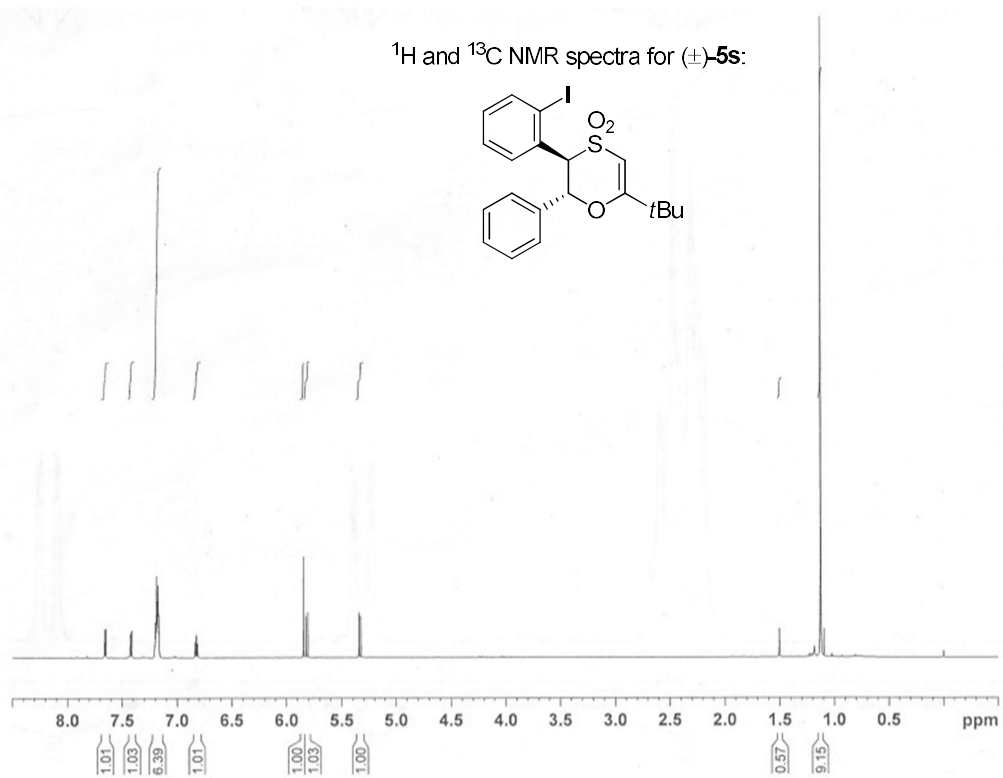
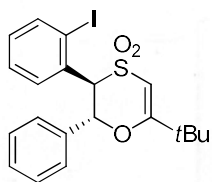
^1H and ^{13}C NMR spectra for ($\pm$)-**5q**
(in DMSO- d_6):



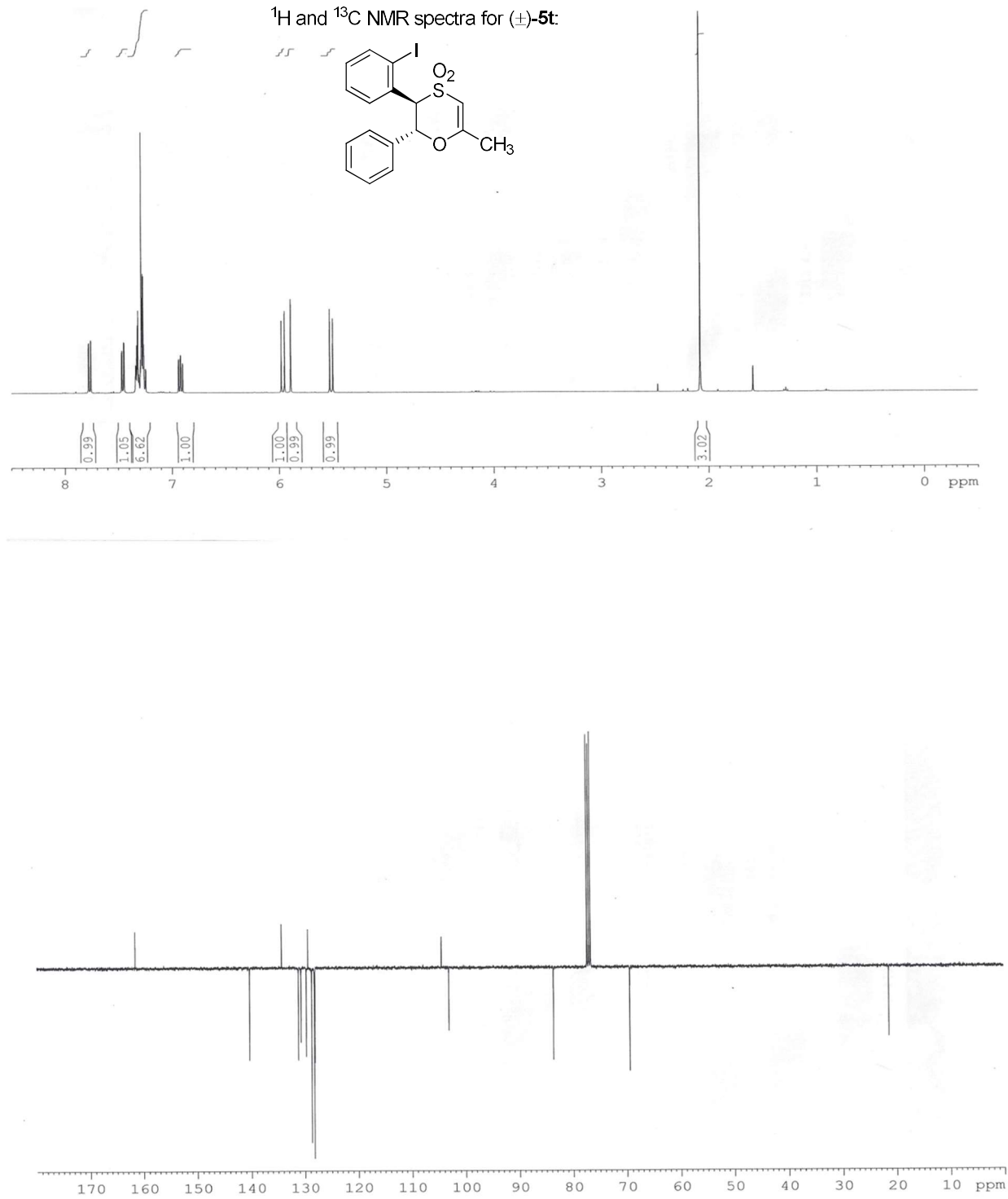
^1H and ^{13}C NMR spectra for ($\pm$)-**5r**:



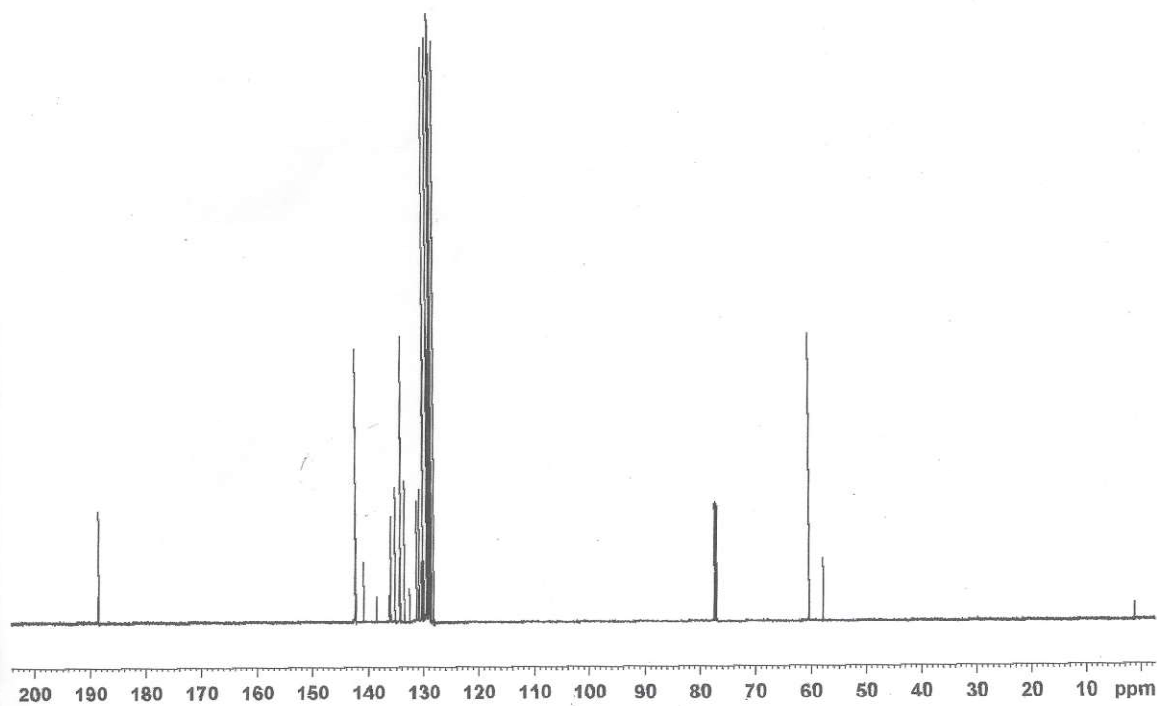
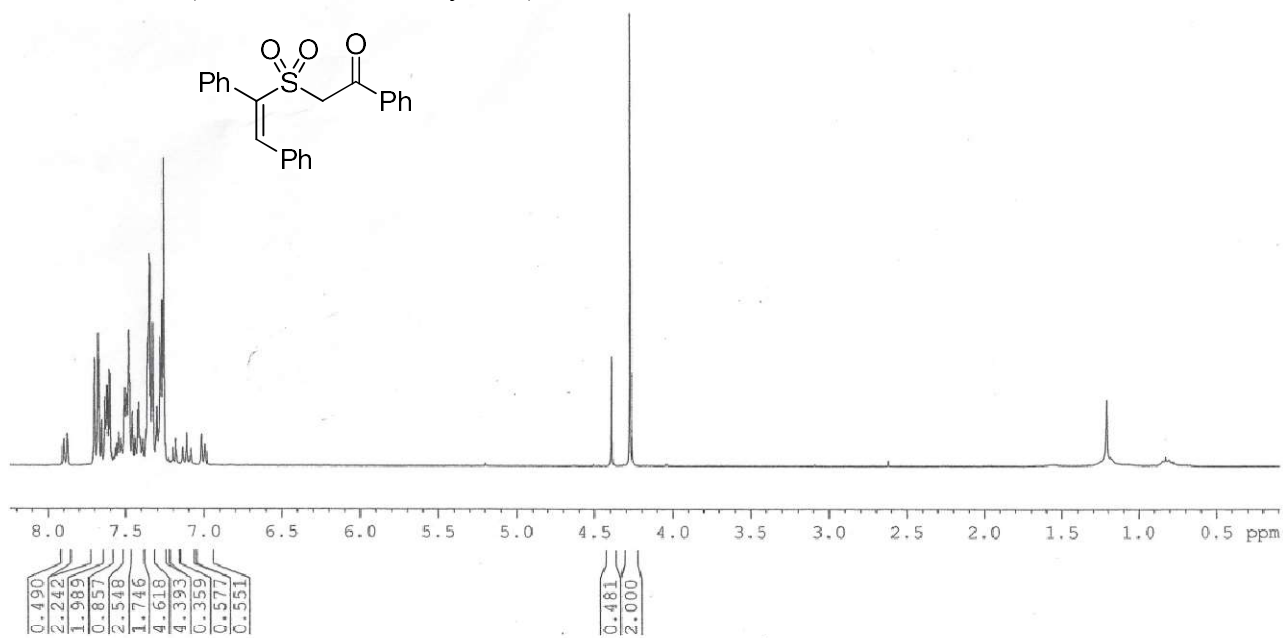
^1H and ^{13}C NMR spectra for ($\pm$)-**5s**:



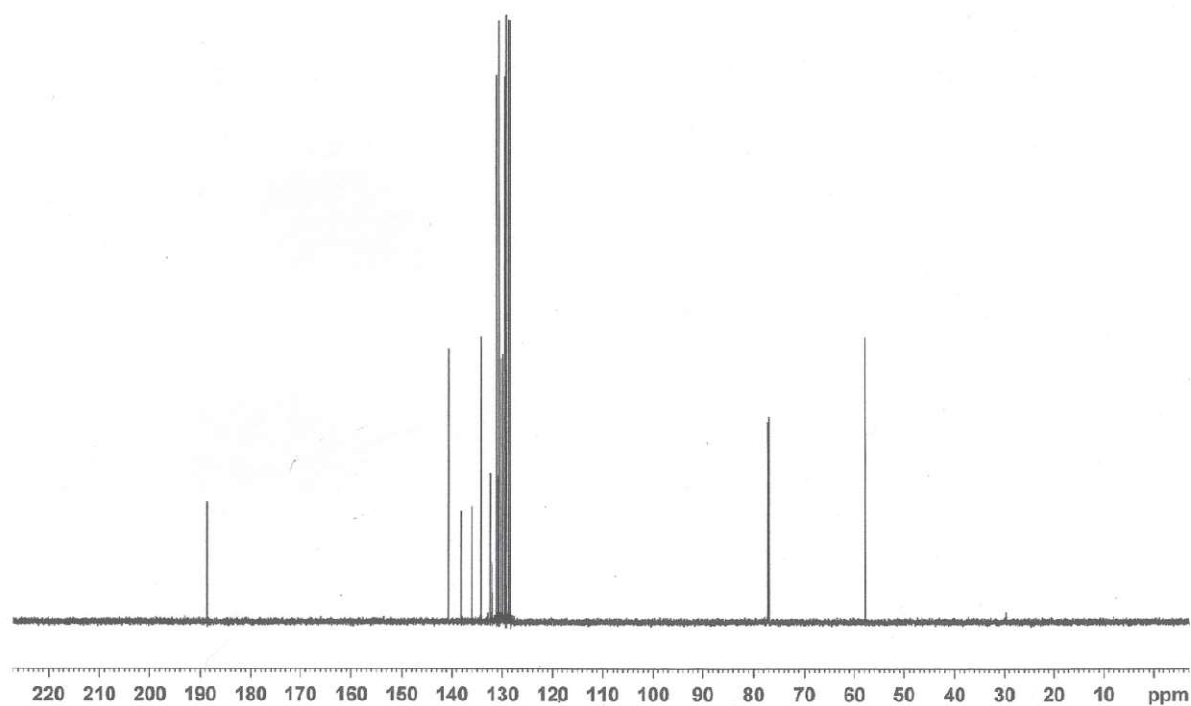
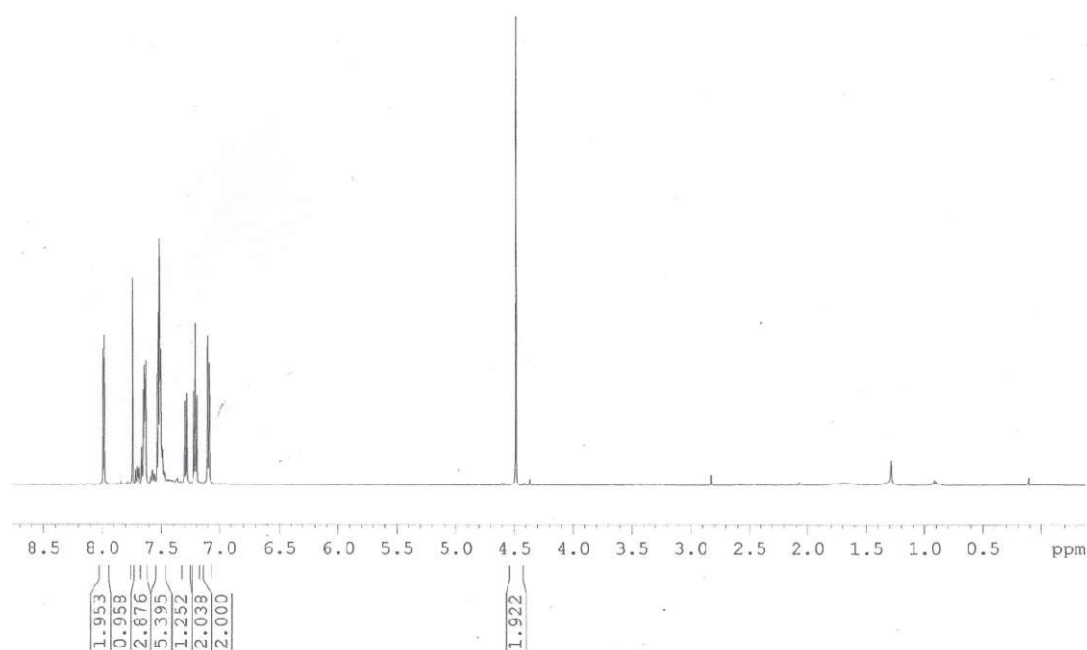
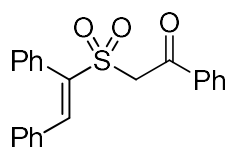
^1H and ^{13}C NMR spectra for ($\pm$)-**5t**:



^1H and ^{13}C NMR spectra for **7Z/E**
mixture (structure drawn is major, **7Z**):



^1H and ^{13}C NMR spectra for **7E**:



Cartesian coordinates and thermochemistry data of structures and transition states

Reactants:

Benzyl Alkynyl Sulfone 6

S	1.90761800	-1.78066300	0.15982200
O	2.47580200	-1.48330200	1.46736600
O	2.13415200	-3.09851700	-0.41656900
C	0.21560000	-1.48753900	0.23328700
C	-0.92379400	-1.09361800	0.19333500
C	2.03160300	0.85172300	-0.63246900
C	2.72312700	1.55416200	0.35557300
C	0.91026100	1.42784100	-1.23130600
C	2.29516600	2.81984500	0.74071600
H	3.59151400	1.10480900	0.82439100
C	0.48354200	2.69433900	-0.84618500
H	0.37122400	0.88241800	-1.99889900
C	1.17431700	3.39031800	0.14230000
H	2.83673900	3.36098000	1.50711500
H	-0.38652100	3.13605000	-1.31729900
H	0.84297000	4.37720700	0.44270100
C	-2.26610600	-0.60912700	0.16091100
C	-3.30566200	-1.42672400	-0.29852100
C	-2.52803900	0.70124500	0.58184500
C	-4.60188600	-0.93122400	-0.33113800
H	-3.08970500	-2.43720000	-0.62244700
C	-3.82812500	1.18601700	0.54131400
H	-1.71195100	1.32247900	0.93161400
C	-4.86333400	0.37176500	0.08707800
H	-5.40888400	-1.56134800	-0.68379300
H	-4.03441900	2.19845100	0.86564200
H	-5.87672200	0.75366500	0.05896100
C	2.46072000	-0.52958300	-1.02419200
H	3.54580800	-0.66074400	-1.02270200
H	2.05408600	-0.84825100	-1.98409700

Zero-point correction=	0.231366
(Hartree/Particle)	
Thermal correction to Energy=	0.247082
Thermal correction to Enthalpy=	0.248027
Thermal correction to Gibbs Free Energy=	0.184354
Sum of electronic and zero-point Energies=	-1126.987555
Sum of electronic and thermal Energies=	-1126.971838
Sum of electronic and thermal Enthalpies=	-1126.970894

Sum of electronic and thermal Free Energies= -1127.034567

Anionic Sulfone Lithiated on One Oxygen (8a)

S	1.55098300	1.93804100	-0.05132900
O	1.92611400	1.93386000	-1.49848100
O	1.68986600	3.22081200	0.64082500
C	-0.15528400	1.57571900	-0.10611900
C	-1.23730000	1.03991900	-0.04411800
C	2.39839100	0.72863700	0.72700400
C	2.19247500	-0.67955700	0.40311900
C	1.58880900	-1.15610500	-0.77869300
C	2.64240200	-1.64660500	1.32657300
C	1.44980700	-2.52110100	-1.01444200
H	1.22026900	-0.45921400	-1.52270700
C	2.50601900	-3.00425700	1.08116900
H	3.10467200	-1.31220400	2.24946900
C	1.90698300	-3.45845600	-0.09438900
H	0.97578300	-2.85016300	-1.93280500
H	2.86556400	-3.71555800	1.81648600
H	1.79793000	-4.51900500	-0.28483900
Li	3.69689100	1.10978600	-1.49630700
H	2.55533900	0.98423900	1.76836700
C	-2.52707000	0.42384100	-0.00764700
C	-3.54124300	0.93956200	0.80887900
C	-2.77090500	-0.71259200	-0.79045500
C	-4.78548900	0.32322800	0.83599400
H	-3.34585200	1.81664600	1.41343700
C	-4.01799300	-1.32173100	-0.75495900
H	-1.97884300	-1.10816900	-1.41510500
C	-5.02611800	-0.80576600	0.05638600
H	-5.56867100	0.72401700	1.46782800
H	-4.20343000	-2.20055000	-1.36042100
H	-5.99790600	-1.28386600	0.08191200

Zero-point correction= 0.220260 (Hartree/Particle)

Thermal correction to Energy= 0.236936

Thermal correction to Enthalpy= 0.237880

Thermal correction to Gibbs Free Energy= 0.173573

Sum of electronic and zero-point Energies= -1133.986103

Sum of electronic and thermal Energies= -1133.969427

Sum of electronic and thermal Enthalpies= -1133.968483

Sum of electronic and thermal Free Energies= -1134.032790

Anionic Sulfone Lithiated on One Oxygen (8b)

S	1.11170100	-1.85819500	-0.24224800
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O	1.53138000	-1.78706200	-1.64411900
C	-0.54791900	-1.31324700	-0.25554900
C	-1.60004800	-0.72413800	-0.16984000
C	2.07380700	-0.95728000	0.79102800
C	2.50524500	0.40392600	0.44566300
C	3.02783000	0.75670700	-0.81127500
C	2.45260300	1.40493800	1.43132100
C	3.45568300	2.05444800	-1.06721200
H	3.09898900	0.00338700	-1.58514500
C	2.90169600	2.69560000	1.17772800
H	2.05273500	1.15999500	2.40999600
C	3.40091500	3.03367900	-0.07757800
H	3.84919300	2.29880600	-2.04770600
H	2.85122600	3.44251700	1.96211000
H	3.74574900	4.04054100	-0.27985600
C	-2.86388500	-0.05895600	-0.09281900
C	-3.81409400	-0.45723900	0.85637700
C	-3.15214700	0.99808600	-0.96605200
C	-5.03721200	0.19645200	0.92655900
H	-3.58585500	-1.27485400	1.52900200
C	-4.37804300	1.64539700	-0.88729700
H	-2.41301000	1.30213200	-1.69701900
C	-5.32136000	1.24705600	0.05713500
H	-5.76987200	-0.11427000	1.66136100
H	-4.59721100	2.46247900	-1.56376100
H	-6.27651200	1.75485300	0.11567800
Li	2.81106000	-3.25386800	1.23295600
H	1.67250600	-1.06763600	1.79820600

Zero-point correction= 0.220398 (Hartree/Particle)

Thermal correction to Energy= 0.237097

Thermal correction to Enthalpy= 0.238041

Thermal correction to Gibbs Free Energy= 0.172578

Sum of electronic and zero-point Energies= -1133.984040

Sum of electronic and thermal Energies= -1133.967341

Sum of electronic and thermal Enthalpies= -1133.966397

Sum of electronic and thermal Free Energies= -1134.031860

Anionic Sulfone Lithiated Bridging Oxygens (8c)

S	1.43578800	1.88477600	0.02587100
O	1.75424100	2.10069900	-1.41549300
O	1.47686000	3.18536200	0.74513500
C	-0.24760000	1.41201600	-0.03073200
C	-1.31735300	0.84991800	0.01235400
C	2.34223600	0.74312900	0.78637100
C	2.35092000	-0.64545700	0.36088400
C	1.95539500	-1.08319400	-0.91898800
C	2.78425200	-1.62830000	1.27375700
C	1.98237300	-2.43305000	-1.25309000
H	1.63439900	-0.36167500	-1.66143400
C	2.81921300	-2.97139900	0.92818500
H	3.09420900	-1.32091300	2.26704800
C	2.41426200	-3.39025100	-0.33901700
H	1.66725900	-2.73672300	-2.24543100
H	3.15965300	-3.69883800	1.65688200
H	2.43748400	-4.43937200	-0.60720700
Li	1.96613800	4.11343300	-1.07974200
H	2.45546200	0.98403500	1.83589700
C	-2.59658400	0.21069200	0.03399000
C	-3.74751000	0.93746600	0.36413900
C	-2.69708500	-1.15119500	-0.27925200
C	-4.98360900	0.30482600	0.37708500
H	-3.66330700	1.98985200	0.60585700
C	-3.93856700	-1.77331100	-0.26597200
H	-1.80155400	-1.70746700	-0.52958500
C	-5.08196700	-1.04851800	0.06203500
H	-5.87198900	0.86931800	0.63285100
H	-4.01318900	-2.82602600	-0.50982200
H	-6.04851300	-1.53763300	0.07260800

Zero-point correction= 0.219506 (Hartree/Particle)

Thermal correction to Energy= 0.236503

Thermal correction to Enthalpy= 0.237448

Thermal correction to Gibbs Free Energy= 0.171357

Sum of electronic and zero-point Energies= -1133.984957

Sum of electronic and thermal Energies= -1133.967960

Sum of electronic and thermal Enthalpies= -1133.967016

Sum of electronic and thermal Free Energies= -1134.033106

Benzaldehyde

C	-1.72443400	1.06258400	-0.00000300
C	-0.35158400	1.28677200	-0.00000100
C	0.53019300	0.20614400	0.00000100
C	0.04140700	-1.10335500	0.00000000
C	-1.32744800	-1.32526700	-0.00000200
C	-2.20891200	-0.24220500	-0.00000300
H	-2.41266100	1.89876300	-0.00000400
H	0.03970100	2.29902600	0.00000000
H	0.74392800	-1.92861400	0.00000100
H	-1.71428000	-2.33702000	-0.00000200
H	-3.27796400	-0.41946700	-0.00000500
C	1.98690500	0.46707300	0.00000300
H	2.27179800	1.53518000	0.00000300
O	2.83409000	-0.39479300	0.00000500

Zero-point correction= 0.110558 (Hartree/Particle)

Thermal correction to Energy= 0.116886

Thermal correction to Enthalpy= 0.117830

Thermal correction to Gibbs Free Energy= 0.079950

Sum of electronic and zero-point Energies= -345.411667

Sum of electronic and thermal Energies= -345.405339

Sum of electronic and thermal Enthalpies= -345.404395

Sum of electronic and thermal Free Energies= -345.442275

Table S8. Important bond lengths and angles for lithiated sulfone **8**.

	C5-S- C3-Ph angle	C3-S- O-Li angle	C6-Ph (Å)	C5- C6 (Å)	C5-S (Å)	S-O (Å)	O-Li (Å)	S-C3 (Å)	C3- Ph (Å)	C3-H (Å)
8a	47.76	- 24.38	1.430	1.209	1.745	1.495, 1.464	1.953	1.669	1.460	1.084
8b	- 74.42	- 30.66	1.430	1.209	1.747	1.492, 1.465	1.979	1.675	1.469	1.090
8c	55.11	-	1.430	1.209	1.749	1.492, 1.487	2.051, 2.105	1.644	1.452	1.083

Pre-Complexes of Lithiated Sulfone and Benzaldehyde:

PC_a

S	-0.46402400	-2.03829100	-0.11896000
O	-0.23259800	-2.33179800	1.32299600
O	-0.51902100	-3.21007700	-0.99914800
C	-2.09628000	-1.39908400	-0.07266000
C	-3.10541200	-0.73469000	-0.12067000
C	0.58628300	-0.90018100	-0.71994900
C	0.74350400	0.41995100	-0.13867900
C	0.52230200	0.72875100	1.21761100
C	1.20959800	1.46146600	-0.96876600
C	0.75258400	2.01214100	1.70596300
H	0.17374500	-0.04151300	1.89433500
C	1.44871400	2.73267900	-0.47185100
H	1.39605400	1.25040600	-2.01688500
C	1.22055800	3.02409200	0.87352000
H	0.56852500	2.21759400	2.75516400
H	1.81794900	3.50411600	-1.13916600
H	1.40524300	4.01826500	1.26245300
Li	1.23525500	-2.73358300	2.41901200
H	0.64795300	-0.99514400	-1.79812200
C	-4.32295200	0.01523500	-0.15938000
C	-5.33381800	-0.32537600	-1.06750300
C	-4.50624800	1.09698600	0.71208400
C	-6.51239300	0.40840100	-1.09803600
H	-5.18651200	-1.16160700	-1.73985800
C	-5.68849900	1.82434900	0.67358100
H	-3.71938800	1.35785300	1.40949400
C	-6.69251800	1.48241000	-0.22942500
H	-7.29183400	0.14182300	-1.80142100
H	-5.82606600	2.66000900	1.34894200
H	-7.61322700	2.05262300	-0.25686700
O	2.72060200	-1.75136000	1.70539800
C	3.05518800	-1.68150600	0.53110200
H	2.87732900	-2.52293600	-0.15326000
C	3.75705900	-0.52233400	-0.03609600
C	4.04586100	0.58785000	0.76045300
C	4.09610600	-0.52979400	-1.38938400
C	4.68263200	1.68581400	0.20117000
H	3.75371700	0.57941700	1.80374200
C	4.73085300	0.57271100	-1.94851600
H	3.84954400	-1.39345400	-1.99892300
C	5.02350600	1.67743900	-1.15138800
H	4.90440700	2.55380400	0.81030400
H	4.99412000	0.57487200	-2.99920100
H	5.51542300	2.53927900	-1.58745300

Zero-point correction=	0.332305 (Hartree/Particle)
Thermal correction to Energy=	0.356841
Thermal correction to Enthalpy=	0.357785
Thermal correction to Gibbs Free Energy=	0.274196
Sum of electronic and zero-point Energies=	-1479.419768
Sum of electronic and thermal Energies=	-1479.395232
Sum of electronic and thermal Enthalpies=	-1479.394288
Sum of electronic and thermal Free Energies=	-1479.477877

PC_b

S	0.37086400	-0.91851200	0.17475600
O	0.62364400	-0.68449700	1.62398100
O	0.98376000	-2.12346300	-0.38839300
C	-1.35815000	-1.21492000	0.17864800
C	-2.56183800	-1.17676500	0.07239300
C	0.71842700	0.41388300	-0.74991700
C	0.17435600	1.73000800	-0.49941500
C	-0.58563500	2.08902900	0.63341300
C	0.43808000	2.74893800	-1.44148600
C	-1.04645000	3.39076100	0.80591900
H	-0.82948300	1.34547000	1.38316700
C	-0.02364900	4.04369100	-1.26053100
H	1.01632500	2.50353900	-2.32691200
C	-0.77130000	4.38145600	-0.13159000
H	-1.63182300	3.62912800	1.68744500
H	0.20088900	4.79699500	-2.00772500
H	-1.13225300	5.39270500	0.00999200
Li	1.54207500	0.49741000	2.76512800
H	1.01258000	0.12988800	-1.75220900
C	-3.98883000	-1.15670000	-0.02895900
C	-4.68644800	0.03264300	0.21989500
C	-4.69263600	-2.31724800	-0.37468600
C	-6.07181800	0.05501600	0.12613800
H	-4.13526500	0.92784300	0.48242400
C	-6.07794300	-2.28400400	-0.46692200
H	-4.14824500	-3.23367900	-0.56656400
C	-6.76937800	-1.10089500	-0.21689000
H	-6.60755800	0.97648100	0.31917500
H	-6.61903600	-3.18343400	-0.73446500
H	-7.85001600	-1.07957400	-0.29003300
O	2.77636500	1.38095600	1.58837700
C	3.14722200	1.12028800	0.45372500
H	3.02196800	1.86436200	-0.34665500

C	3.86076700	-0.11364500	0.07628500
C	4.18500400	-1.08214800	1.02843500
C	4.21737300	-0.29663300	-1.26089800
C	4.85154400	-2.23548800	0.63803900
H	3.91994800	-0.92475600	2.06714800
C	4.88247700	-1.45147000	-1.65080000
H	3.95623600	0.46241900	-1.99156500
C	5.19612900	-2.42123900	-0.70032400
H	5.10420700	-2.99102000	1.37193300
H	5.15413100	-1.59946300	-2.68870000
H	5.71336100	-3.32427500	-1.00246400

Zero-point correction= 0.332978 (Hartree/Particle)
 Thermal correction to Energy= 0.357240
 Thermal correction to Enthalpy= 0.358184
 Thermal correction to Gibbs Free Energy= 0.275189
 Sum of electronic and zero-point Energies= -1479.414703
 Sum of electronic and thermal Energies= -1479.390441
 Sum of electronic and thermal Enthalpies= -1479.389497
 Sum of electronic and thermal Free Energies= -1479.472492

PC_c

S	-0.27352200	-1.48754800	0.02540500
O	0.25245200	-1.41189900	1.39225200
O	-0.35707000	-2.85047800	-0.57112500
C	-1.96825000	-1.06105900	0.20845600
C	-3.08077800	-0.58717200	0.19487100
C	0.50524300	-0.49088100	-1.04555500
C	0.86546900	0.88689800	-0.76534900
C	1.06526400	1.41895000	0.52423400
C	1.11462800	1.74005300	-1.85997000
C	1.48448200	2.73217600	0.69590100
H	0.91573000	0.78779400	1.39020500
C	1.54589600	3.04718700	-1.67934600
H	0.97254200	1.35696400	-2.86569800
C	1.73384600	3.55934600	-0.39698600
H	1.63499500	3.10898300	1.70213100
H	1.73263500	3.67099100	-2.54685000
H	2.06983900	4.57932000	-0.25340500
Li	1.02754100	-4.15267700	-0.52606700
H	0.26463300	-0.76711700	-2.06596100
C	-4.41488700	-0.07111300	0.20431000
C	-4.78806500	0.90171800	1.14101700
C	-5.35524300	-0.53910700	-0.72307200

C	-6.08587900	1.39582400	1.14666300
H	-4.05759400	1.26081900	1.85555900
C	-6.65074400	-0.03933100	-0.70872700
H	-5.06204300	-1.29089000	-1.44558000
C	-7.01868500	0.92744500	0.22426500
H	-6.36996600	2.14785500	1.87266200
H	-7.37434400	-0.40482800	-1.42722500
H	-8.03020200	1.31521200	0.23224500
O	2.59834600	-3.06022800	-0.26155300
C	2.91452400	-2.00329600	-0.79422200
H	2.79371800	-1.87143700	-1.87910000
C	3.54737300	-0.88202800	-0.08810300
C	3.69635000	-0.89969800	1.30086500
C	3.98086600	0.21966400	-0.82849400
C	4.29230000	0.17785200	1.94046300
H	3.33282200	-1.75386600	1.85931200
C	4.57748700	1.29725600	-0.18635700
H	3.83665700	0.23269600	-1.90399000
C	4.73472900	1.27295400	1.19669200
H	4.40901000	0.17297500	3.01760800
H	4.90577500	2.15711600	-0.75735600
H	5.19415400	2.11524600	1.70122800

Zero-point correction=	0.332322 (Hartree/Particle)
Thermal correction to Energy=	0.356808
Thermal correction to Enthalpy=	0.357752
Thermal correction to Gibbs Free Energy=	0.274369
Sum of electronic and zero-point Energies=	-1479.418236
Sum of electronic and thermal Energies=	-1479.393751
Sum of electronic and thermal Enthalpies=	-1479.392806
Sum of electronic and thermal Free Energies=	-1479.476189

PC_d

S	0.43899200	-1.47303100	-0.54799600
O	0.18665500	-1.29541800	-1.98371300
O	0.39964300	-2.87558700	-0.04586900
C	2.13422700	-1.05593800	-0.38259200
C	3.22288100	-0.58243300	-0.15308400
C	-0.54021100	-0.55017400	0.41305700
C	-0.86602600	0.84299400	0.18934800
C	-0.64647400	1.54438600	-1.01294500
C	-1.51802000	1.53582400	1.23042000
C	-1.06336200	2.86353600	-1.15543700

H	-0.16216500	1.04706600	-1.84407600
C	-1.94014500	2.84724800	1.07533200
H	-1.70550500	1.01866700	2.16604300
C	-1.71786500	3.52772600	-0.12122700
H	-0.87864000	3.37519100	-2.09395600
H	-2.45034000	3.34216200	1.89478400
H	-2.04706200	4.55257600	-0.24360500
Li	-1.00925800	-4.04715300	0.41215400
H	-0.59431800	-0.95020700	1.41834000
C	4.53264600	-0.06153700	0.09001700
C	5.05181400	0.94628100	-0.73330200
C	5.30259600	-0.55873700	1.14977100
C	6.32549700	1.44612400	-0.49645300
H	4.45230300	1.32765300	-1.55076900
C	6.57591600	-0.05340900	1.37723800
H	4.89677800	-1.33759700	1.78363900
C	7.08947000	0.94822200	0.55662200
H	6.72276100	2.22529300	-1.13549200
H	7.16840700	-0.44175400	2.19668700
H	8.08313500	1.34004800	0.73733400
O	-2.67952100	-3.04571300	0.35312700
C	-2.79793200	-2.06018600	-0.36672200
H	-2.28805200	-2.01910900	-1.34087000
C	-3.65756800	-0.90924200	-0.06172400
C	-4.35651100	-0.82672000	1.14536400
C	-3.73704200	0.12676600	-0.99455100
C	-5.13907000	0.28834600	1.40945100
H	-4.27474300	-1.63628600	1.86159500
C	-4.51985600	1.24287800	-0.72723500
H	-3.17021200	0.05983400	-1.91753400
C	-5.22098700	1.32036400	0.47286700
H	-5.68409000	0.36068900	2.34297400
H	-4.57364900	2.05344800	-1.44354700
H	-5.82879600	2.19210200	0.68627100

Zero-point correction=	0.332114 (Hartree/Particle)
Thermal correction to Energy=	0.356788
Thermal correction to Enthalpy=	0.357732
Thermal correction to Gibbs Free Energy=	0.273902
Sum of electronic and zero-point Energies=	-1479.418302
Sum of electronic and thermal Energies=	-1479.393628
Sum of electronic and thermal Enthalpies=	-1479.392684
Sum of electronic and thermal Free Energies=	-1479.476513

S	0.35147000	-2.15470400	-0.35884300
O	0.58819100	-3.31289800	-1.23398100
O	0.09507000	-2.57334600	1.04864700
C	1.85793300	-1.28757900	-0.34675200
C	2.89352400	-0.67372900	-0.25928000
C	-0.72443200	-0.96963400	-0.84660800
C	-2.15754700	-1.03620800	-0.63818100
C	-2.79775000	-1.70170700	0.42743700
C	-2.97868000	-0.28869300	-1.51142500
C	-4.17669100	-1.61748000	0.59770000
H	-2.21361200	-2.28701400	1.12417900
C	-4.34944300	-0.20496700	-1.32840700
H	-2.51516400	0.24160800	-2.33707000
C	-4.96796700	-0.87045700	-0.26960300
H	-4.63581000	-2.14514600	1.42719500
H	-4.94164300	0.38757900	-2.01773400
H	-6.03998100	-0.80781100	-0.12645300
Li	0.06077200	-1.69068300	2.72807400
H	-0.36175100	-0.50006300	-1.75599100
C	4.11755200	0.06353600	-0.17963700
C	5.32404100	-0.59921000	0.07753200
C	4.10722600	1.45287300	-0.35805700
C	6.50610400	0.12534100	0.15579600
H	5.32456900	-1.67378900	0.21276000
C	5.29524100	2.16767000	-0.28181600
H	3.16982200	1.95827200	-0.55749400
C	6.49398500	1.50655100	-0.02435800
H	7.43826500	-0.38874200	0.35550000
H	5.28573700	3.24151400	-0.42280400
H	7.41876000	2.06761900	0.03552800
O	-0.62343300	0.03621200	2.23959000
C	-0.40906400	0.76082100	1.27426100
H	0.59459200	0.82108900	0.83054300
C	-1.42029400	1.67342800	0.71721100
C	-2.70704600	1.71761000	1.25587500
C	-1.08889500	2.46565900	-0.38262200
C	-3.65789500	2.56089300	0.69699600
H	-2.94802100	1.07990700	2.09793700
C	-2.04216700	3.30654600	-0.94299900
H	-0.08925800	2.40554500	-0.80267800
C	-3.32567800	3.35309100	-0.40077400
H	-4.66059700	2.59510800	1.10597200
H	-1.79127100	3.92012300	-1.79983000
H	-4.07143000	4.00563400	-0.84006500

Zero-point correction=

0.331976 (Hartree/Particle)

Thermal correction to Energy=	0.356538
Thermal correction to Enthalpy=	0.357482
Thermal correction to Gibbs Free Energy=	0.274390
Sum of electronic and zero-point Energies=	-1479.411559
Sum of electronic and thermal Energies=	-1479.386997
Sum of electronic and thermal Enthalpies=	-1479.386053
Sum of electronic and thermal Free Energies=	-1479.469145

PC_f

S	0.19012800	1.49426400	1.95137700
O	0.15389400	0.77127100	3.25519200
O	0.56385700	2.91113400	2.01426000
C	1.58251100	0.79320800	1.13829100
C	2.46740600	0.29847300	0.47983300
C	-1.20437200	1.14643500	1.13885700
C	-1.55288800	1.64349600	-0.16907100
C	-0.66112700	2.32912500	-1.01981600
C	-2.85154700	1.39567300	-0.66092200
C	-1.05697300	2.74254000	-2.28670400
H	0.34815200	2.54507800	-0.68668800
C	-3.23930500	1.81618600	-1.92431800
H	-3.55294800	0.85159800	-0.03499000
C	-2.34633300	2.49451700	-2.75342400
H	-0.34600800	3.26633400	-2.91634900
H	-4.24674200	1.60641700	-2.26766000
H	-2.64842000	2.82217400	-3.74063000
Li	0.40767300	-1.10707200	3.53612600
H	-1.85809500	0.49236100	1.69635500
C	3.54831400	-0.28579900	-0.25469500
C	3.62823900	-1.67688400	-0.39930600
C	4.53431100	0.53076400	-0.82358600
C	4.68393500	-2.24047400	-1.10392400
H	2.86476900	-2.30460100	0.04484000
C	5.58565700	-0.04208500	-1.52698300
H	4.46819400	1.60553900	-0.70712800
C	5.66277400	-1.42581400	-1.66817400
H	4.74305300	-3.31653500	-1.21278300
H	6.34678600	0.59222900	-1.96463900
H	6.48506600	-1.86876300	-2.21700000
O	-0.26264000	-1.89410000	1.89859400
C	-0.55609400	-1.64026800	0.73968700
H	0.19890300	-1.22378200	0.05521100
C	-1.87563900	-1.90068400	0.14871500
C	-2.93714800	-2.36395800	0.93467500

C	-2.06140800	-1.65039600	-1.21087300
C	-4.17626700	-2.57900600	0.35350400
H	-2.77487700	-2.54390400	1.99115500
C	-3.30310400	-1.88062500	-1.79459600
H	-1.23782700	-1.26516300	-1.80387400
C	-4.35636400	-2.34131700	-1.01257700
H	-5.00513500	-2.93242000	0.95461300
H	-3.45150900	-1.68532500	-2.84944500
H	-5.32678500	-2.51332400	-1.46332400

Zero-point correction=	0.331597 (Hartree/Particle)
Thermal correction to Energy=	0.356553
Thermal correction to Enthalpy=	0.357497
Thermal correction to Gibbs Free Energy=	0.271994
Sum of electronic and zero-point Energies=	-1479.414971
Sum of electronic and thermal Energies=	-1479.390016
Sum of electronic and thermal Enthalpies=	-1479.389071
Sum of electronic and thermal Free Energies=	-1479.474574

PC_g

S	2.39430200	-1.82562800	-0.44613900
O	2.83060700	-2.14554000	-1.80985800
O	2.61887700	-2.90017500	0.56573100
C	0.65228100	-1.73626600	-0.63005100
C	-0.49884600	-1.42462900	-0.82727000
C	2.96762000	-0.40377800	0.17930400
C	2.62925100	0.90099800	-0.33405000
C	1.93471500	1.12948000	-1.54185500
C	2.96372900	2.03821500	0.43587500
C	1.56533800	2.41415900	-1.92426300
H	1.68287000	0.29608300	-2.18783500
C	2.60231800	3.31749500	0.03893800
H	3.51307500	1.90028800	1.36231200
C	1.88566800	3.52095200	-1.14055400
H	1.02310600	2.55008000	-2.85406100
H	2.87591700	4.16331900	0.66046900
H	1.59601600	4.51845800	-1.44723100
Li	1.81154400	-2.93245000	2.30353900
H	3.29124300	-0.52302600	1.20384300
C	-1.86268700	-1.06626900	-1.06543000
C	-2.90113400	-1.94687900	-0.73545700
C	-2.15714400	0.18195600	-1.62574600
C	-4.21890100	-1.57619100	-0.96345200
H	-2.66525100	-2.91045100	-0.29999400

C	-3.47960900	0.54183000	-1.85335300
H	-1.34658500	0.86114800	-1.86506400
C	-4.51072400	-0.33242500	-1.52109600
H	-5.02060200	-2.25764400	-0.70529000
H	-3.70515600	1.51098400	-2.28226100
H	-5.54106100	-0.04658800	-1.69643200
O	0.68810300	-1.37279100	2.54188400
C	0.58036100	-0.19393600	2.24600600
H	1.46836200	0.45291300	2.20659900
C	-0.69006500	0.46317300	1.92614800
C	-1.91131100	-0.18684700	2.13051400
C	-0.65253900	1.75676300	1.39681400
C	-3.09405400	0.46709000	1.82287400
H	-1.91515100	-1.19543700	2.52815200
C	-1.84072100	2.40227900	1.07599900
H	0.30525800	2.23971100	1.22332600
C	-3.05635600	1.75959400	1.29697600
H	-4.04554600	-0.02725400	1.97677300
H	-1.82029100	3.39974300	0.65397800
H	-3.98350600	2.26254600	1.04704400

Zero-point correction=	0.332626 (Hartree/Particle)
Thermal correction to Energy=	0.356856
Thermal correction to Enthalpy=	0.357800
Thermal correction to Gibbs Free Energy=	0.277639
Sum of electronic and zero-point Energies=	-1479.419222
Sum of electronic and thermal Energies=	-1479.394992
Sum of electronic and thermal Enthalpies=	-1479.394048
Sum of electronic and thermal Free Energies=	-1479.474209

PC_h

S	1.02069500	-1.61642400	-0.40629400
O	1.26282700	-1.20413100	-1.82242800
O	1.26519200	-3.06027500	-0.24464000
C	-0.66162400	-1.36837400	-0.09562400
C	-1.84431200	-1.23857000	0.10068500
C	1.72606500	-0.54737300	0.67908500
C	3.15556800	-0.33404200	0.70751200
C	4.05377900	-0.76707300	-0.29080100
C	3.69860900	0.41784000	1.77345600
C	5.40875400	-0.46281500	-0.21869000
H	3.69559700	-1.36356500	-1.12210400
C	5.05150100	0.71648300	1.83642000
H	3.03453700	0.76549000	2.55896600

C	5.92453500	0.28174400	0.83878300
H	6.07023000	-0.81977700	-1.00068900
H	5.42886200	1.29440700	2.67306500
H	6.98111400	0.51411300	0.88862300
Li	1.94419800	0.23050600	-2.83388100
H	1.14597400	-0.46502200	1.59010500
C	-3.24273000	-1.03443100	0.31636600
C	-3.72060800	-0.75332200	1.60137500
C	-4.12461700	-1.05461800	-0.77016800
C	-5.06965200	-0.48514000	1.79171100
H	-3.02953500	-0.73183400	2.43532900
C	-5.47253700	-0.78711800	-0.56945400
H	-3.74434700	-1.26649300	-1.76211600
C	-5.94592900	-0.49777400	0.70837700
H	-5.43767100	-0.26242900	2.78586600
H	-6.15349300	-0.79993600	-1.41174900
H	-6.99717700	-0.28454900	0.86044300
O	1.97435000	1.66854000	-1.58068300
C	1.37501800	1.84920100	-0.52799200
H	1.93577400	2.08389500	0.38749700
C	-0.09422000	1.93548400	-0.42278400
C	-0.90575000	1.82819100	-1.55380600
C	-0.66891300	2.15261200	0.83114600
C	-2.28554200	1.92497200	-1.42660900
H	-0.45125500	1.67910100	-2.52626500
C	-2.04826700	2.24896300	0.95734900
H	-0.02831600	2.23023500	1.70431200
C	-2.85609400	2.13208800	-0.17222800
H	-2.91921200	1.83421700	-2.30097100
H	-2.49694000	2.40458100	1.93117600
H	-3.93500500	2.18419300	-0.07179100

Zero-point correction= 0.332106 (Hartree/Particle)
 Thermal correction to Energy= 0.356535
 Thermal correction to Enthalpy= 0.357479
 Thermal correction to Gibbs Free Energy= 0.276344
 Sum of electronic and zero-point Energies= -1479.411701
 Sum of electronic and thermal Energies= -1479.387272
 Sum of electronic and thermal Enthalpies= -1479.386328
 Sum of electronic and thermal Free Energies= -1479.467463

Transition States for Benzaldehyde Addition to the Lithiated Sulfone:

PC_a[‡]

S	-0.32358500	-1.92855100	0.14443100
O	-0.16481300	-2.20032600	1.59625500
O	-0.24511300	-3.09791500	-0.73282400
C	-1.96104300	-1.34052600	0.04365500
C	-3.00331800	-0.75074800	-0.11574500
C	0.74344600	-0.73799100	-0.38218500
C	0.74258500	0.59635900	0.19782700
C	0.38979200	0.88508200	1.52892400
C	1.20199700	1.66302000	-0.59952100
C	0.48098600	2.18314900	2.02444600
H	0.03795300	0.09367500	2.17870700
C	1.29883200	2.95161000	-0.09666600
H	1.49685000	1.46077700	-1.62467300
C	0.93594500	3.22504400	1.22196200
H	0.19551700	2.37773700	3.05239800
H	1.66083000	3.74830900	-0.73713800
H	1.00723300	4.23196600	1.61523400
Li	1.37578500	-2.44015700	2.68659100
H	0.84057900	-0.80973500	-1.46092000
C	-4.25590200	-0.08210800	-0.28702100
C	-5.30144000	-0.71099400	-0.97490200
C	-4.43585300	1.20666300	0.23164400
C	-6.51341100	-0.05350400	-1.13868300
H	-5.15468100	-1.70724500	-1.37350500
C	-5.65214200	1.85493700	0.06256000
H	-3.62121900	1.68745800	0.75976800
C	-6.69091600	1.22766600	-0.62138400
H	-7.32065600	-0.54174300	-1.67080300
H	-5.78906400	2.85157000	0.46395300
H	-7.63807300	1.73708600	-0.75171200
O	2.74520800	-1.62742500	1.67753400
C	2.83950700	-1.61978100	0.44237700
H	2.59158200	-2.51450500	-0.14437800
C	3.61384000	-0.57978400	-0.27396100
C	4.12194700	0.51776100	0.42019500
C	3.83116300	-0.69806800	-1.64779400
C	4.84875700	1.49071700	-0.25684900
H	3.93540800	0.59767200	1.48496900
C	4.55365400	0.27607400	-2.32486900
H	3.42304800	-1.55088900	-2.18202900
C	5.06349900	1.37179300	-1.62777200
H	5.24186300	2.34533600	0.28108500
H	4.72182400	0.18466000	-3.39124700
H	5.62719600	2.13224900	-2.15552300

Zero-point correction=	0.332156 (Hartree/Particle)
Thermal correction to Energy=	0.355897
Thermal correction to Enthalpy=	0.356841
Thermal correction to Gibbs Free Energy=	0.273705
Sum of electronic and zero-point Energies=	-1479.418691
Sum of electronic and thermal Energies=	-1479.394949
Sum of electronic and thermal Enthalpies=	-1479.394005
Sum of electronic and thermal Free Energies=	-1479.477142

Imaginary Frequency	-116.23 cm ⁻¹
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PC_b[‡]

S	0.45861800	-0.88054800	0.44854000
O	0.68026600	-0.56173800	1.88321400
O	1.11314800	-2.08901400	-0.04741500
C	-1.25906800	-1.18226300	0.38881100
C	-2.45182600	-1.19004200	0.19611900
C	0.82315300	0.43986900	-0.53100700
C	0.11346100	1.70339600	-0.39400200
C	-0.60966500	2.10090000	0.74636600
C	0.20162900	2.62442900	-1.45746200
C	-1.21666800	3.35202900	0.80747700
H	-0.71548100	1.42733500	1.58810900
C	-0.39971300	3.87240400	-1.38645700
H	0.75049500	2.34237900	-2.35060600
C	-1.11692600	4.24899300	-0.25107800
H	-1.77354800	3.62518700	1.69701400
H	-0.31214600	4.55463000	-2.22459400
H	-1.58983300	5.22187100	-0.19584600
Li	1.77449800	0.68656900	2.81514800
H	1.04506200	0.09307300	-1.53477300
C	-3.86777300	-1.21479900	-0.00287500
C	-4.61217100	-0.04032600	0.16802400
C	-4.51113800	-2.40294700	-0.37134900
C	-5.98703700	-0.06032300	-0.02545900
H	-4.10535900	0.87535100	0.44866000
C	-5.88648000	-2.41160600	-0.56284500
H	-3.92899500	-3.30665100	-0.50312700
C	-6.62548200	-1.24343900	-0.39040400
H	-6.56070800	0.84883000	0.10697000
H	-6.38247000	-3.33146700	-0.84750100
H	-7.69818900	-1.25489300	-0.54129900
O	2.79512000	1.48703700	1.46021000
C	2.97481600	1.14708700	0.28423700

H	2.82361900	1.87815100	-0.52196400
C	3.75093400	-0.06055700	-0.09846200
C	4.24187900	-0.93715500	0.86852300
C	4.01918700	-0.29482800	-1.44836800
C	4.97807200	-2.05230500	0.48492900
H	4.05363700	-0.73927300	1.91718300
C	4.75453200	-1.40794400	-1.83216000
H	3.63813800	0.39542900	-2.19509600
C	5.23086200	-2.29131100	-0.86384600
H	5.35742700	-2.73476400	1.23611700
H	4.95775300	-1.59004400	-2.88057900
H	5.80347100	-3.16193400	-1.16109600

Zero-point correction= 0.332844 (Hartree/Particle)
 Thermal correction to Energy= 0.356269
 Thermal correction to Enthalpy= 0.357214
 Thermal correction to Gibbs Free Energy= 0.276344
 Sum of electronic and zero-point Energies= -1479.413623
 Sum of electronic and thermal Energies= -1479.390197
 Sum of electronic and thermal Enthalpies= -1479.389253
 Sum of electronic and thermal Free Energies= -1479.470123

Imaginary Frequency -127.84 cm⁻¹

PC_c[‡]

S	-0.07261200	-1.71012100	0.15229300
O	0.48048100	-1.56997400	1.49871100
O	-0.10267500	-3.08477500	-0.40472200
C	-1.74900100	-1.26053300	0.29261700
C	-2.84781900	-0.75878300	0.25990800
C	0.68937100	-0.70476000	-0.98203600
C	0.70555700	0.74369800	-0.76811000
C	0.86462400	1.34542800	0.49275300
C	0.65578900	1.58387400	-1.89333900
C	0.95560900	2.72667700	0.61291500
H	0.93958000	0.72365400	1.37594200
C	0.76359800	2.96384700	-1.76844300
H	0.53695600	1.14110000	-2.87718700
C	0.91078800	3.54719800	-0.51219600
H	1.07890100	3.16551300	1.59696100
H	0.72623900	3.58554300	-2.65599100
H	0.99122400	4.62300300	-0.41200100
Li	1.48462600	-4.13938700	-0.63616200
H	0.36580400	-1.02564800	-1.96943300

C	-4.16195500	-0.19570300	0.25053600
C	-4.44703100	0.92624500	1.03954300
C	-5.16397500	-0.76160900	-0.54814100
C	-5.72353400	1.47230600	1.02670300
H	-3.66640900	1.35893200	1.65321100
C	-6.43737700	-0.20816200	-0.55263500
H	-4.93605600	-1.62846900	-1.15609100
C	-6.71898900	0.90731800	0.23279600
H	-5.94188900	2.33997900	1.63709800
H	-7.21103500	-0.64750200	-1.17035900
H	-7.71374100	1.33627600	0.22587800
O	2.76963600	-2.78873500	-0.61016400
C	2.81810000	-1.60388600	-1.00060000
H	2.76330300	-1.38085600	-2.07473700
C	3.44891500	-0.53528300	-0.18652900
C	3.62938400	-0.69654200	1.18752800
C	3.86713200	0.64156500	-0.80810800
C	4.22267300	0.31538200	1.93202700
H	3.28239600	-1.60868800	1.65757300
C	4.46640700	1.65219400	-0.06395500
H	3.71544200	0.76587300	-1.87576000
C	4.64272100	1.49003900	1.30756700
H	4.35758700	0.19326700	3.00049200
H	4.78929700	2.56512900	-0.55046600
H	5.10485100	2.27780400	1.89125700

Zero-point correction=	0.332788 (Hartree/Particle)
Thermal correction to Energy=	0.356146
Thermal correction to Enthalpy=	0.357090
Thermal correction to Gibbs Free Energy=	0.276726
Sum of electronic and zero-point Energies=	-1479.415598
Sum of electronic and thermal Energies=	-1479.392240
Sum of electronic and thermal Enthalpies=	-1479.391296
Sum of electronic and thermal Free Energies=	-1479.471660

Imaginary Frequency	-136.72 cm ⁻¹
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PC_d⁺

S	0.31750100	-1.75508600	-0.61184400
O	0.13933700	-1.71521800	-2.06584700
O	0.20634100	-3.09366800	0.02068100

C	1.97783300	-1.28823900	-0.35926900
C	3.02488100	-0.74215400	-0.10108300
C	-0.71944900	-0.70508300	0.19758500
C	-0.75581200	0.71954200	-0.11124200
C	-0.52391600	1.26181700	-1.38837500
C	-1.14107000	1.60375900	0.91331600
C	-0.66457300	2.62693600	-1.61665900
H	-0.24634300	0.60896500	-2.20672300
C	-1.29519200	2.96183300	0.67450100
H	-1.33448000	1.20624000	1.90439600
C	-1.05458800	3.48762100	-0.59384600
H	-0.47637800	3.01871500	-2.61020900
H	-1.60289900	3.61460900	1.48396300
H	-1.17047600	4.54833500	-0.78134300
Li	-1.37567900	-4.14890200	0.29199300
H	-0.75631400	-0.97905400	1.24802900
C	4.28483300	-0.12771300	0.18040900
C	4.77062800	0.88570700	-0.65623100
C	5.03322800	-0.53328800	1.29287600
C	5.99268500	1.48348500	-0.37874500
H	4.18577600	1.19520400	-1.51372700
C	6.25493900	0.07000100	1.56028100
H	4.65154000	-1.31656100	1.93609200
C	6.73598900	1.07749500	0.72722500
H	6.36544700	2.26728100	-1.02672000
H	6.83230800	-0.24565700	2.42059900
H	7.68912100	1.54643300	0.93986000
O	-2.75593200	-2.85365400	0.32062600
C	-2.78888300	-1.79136400	-0.32116800
H	-2.47496200	-1.76603100	-1.37405600
C	-3.57913400	-0.62005200	0.12152600
C	-4.05281100	-0.53319300	1.43163900
C	-3.84136500	0.40885900	-0.78367900
C	-4.78300900	0.57877300	1.83173900
H	-3.83808800	-1.33941200	2.12391700
C	-4.57711700	1.51898600	-0.38411200
H	-3.45903900	0.34002000	-1.79694800
C	-5.04693600	1.60467100	0.92377600
H	-5.14849900	0.64970000	2.84948000
H	-4.77800400	2.31792400	-1.08797200
H	-5.61663400	2.47131100	1.23842800

Zero-point correction=	0.332366 (Hartree/Particle)
Thermal correction to Energy=	0.356005
Thermal correction to Enthalpy=	0.356949
Thermal correction to Gibbs Free Energy=	0.275441
Sum of electronic and zero-point Energies=	-1479.416936

Sum of electronic and thermal Energies=	-1479.393297
Sum of electronic and thermal Enthalpies=	-1479.392353
Sum of electronic and thermal Free Energies=	-1479.473860

Imaginary Frequency	-115.53 cm ⁻¹
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PC_e[‡]

S	0.33693100	-2.09554500	-0.33189500
O	0.50986600	-3.22645600	-1.25453400
O	0.10796900	-2.55376700	1.06666900
C	1.85540500	-1.25456500	-0.33301200
C	2.90504700	-0.66456500	-0.25423800
C	-0.72886300	-0.85988200	-0.74640200
C	-2.16907600	-1.00411500	-0.60954700
C	-2.81012300	-1.70688500	0.42958800
C	-2.98947500	-0.28757800	-1.50571300
C	-4.19638500	-1.68845000	0.55372500
H	-2.22113200	-2.26627500	1.14374200
C	-4.36855900	-0.26612800	-1.36767800
H	-2.52176000	0.26936500	-2.31113800
C	-4.98933100	-0.96873300	-0.33499500
H	-4.65961500	-2.24270700	1.36310100
H	-4.96469300	0.30417000	-2.07196000
H	-6.06731700	-0.95577100	-0.22775500
Li	0.05631500	-1.66761600	2.74924700
H	-0.36086200	-0.36197000	-1.63972100
C	4.14561500	0.04500900	-0.18365100
C	5.34543700	-0.65138300	0.00691500
C	4.15731200	1.44049700	-0.30362500
C	6.54371200	0.04680000	0.07741500
H	5.32827600	-1.73048000	0.09742900
C	5.36138000	2.12860600	-0.23538500
H	3.22462000	1.97168900	-0.45116500
C	6.55381900	1.43437700	-0.04429400
H	7.47103800	-0.49282600	0.22545400
H	5.36926500	3.20744300	-0.33072200
H	7.49118400	1.97476100	0.00962700
O	-0.63358700	0.03446200	2.23275400
C	-0.41928400	0.73922000	1.24527900
H	0.59444900	0.83570400	0.83361500
C	-1.42940400	1.66772700	0.70075700
C	-2.71554700	1.70505200	1.23976900
C	-1.09705900	2.48886200	-0.37749300
C	-3.66467300	2.56616500	0.70271000
H	-2.95786300	1.04881600	2.06711800

C	-2.04680400	3.34828500	-0.91515500
H	-0.09752600	2.43772000	-0.79941400
C	-3.33132500	3.38610800	-0.37330400
H	-4.66660300	2.59360400	1.11451100
H	-1.79205200	3.98444600	-1.75436400
H	-4.07415900	4.05342400	-0.79489300

Zero-point correction= 0.331680 (Hartree/Particle)
 Thermal correction to Energy= 0.355468
 Thermal correction to Enthalpy= 0.356412
 Thermal correction to Gibbs Free Energy= 0.274627
 Sum of electronic and zero-point Energies= -1479.411791
 Sum of electronic and thermal Energies= -1479.388003
 Sum of electronic and thermal Enthalpies= -1479.387059
 Sum of electronic and thermal Free Energies= -1479.468844

Imaginary Frequency -89.00 cm⁻¹

PC_f[‡]

S	0.18415300	1.41540600	1.96013900
O	0.15579200	0.69515000	3.26053600
O	0.43021000	2.85699100	2.04625600
C	1.59118900	0.80077200	1.13895300
C	2.49842800	0.32217500	0.50227000
C	-1.15359600	0.90485000	1.07448800
C	-1.53241400	1.52867000	-0.17899000
C	-0.62533600	2.17740200	-1.03940200
C	-2.86717800	1.41213000	-0.61194700
C	-1.04162800	2.68455700	-2.26471800
H	0.41300300	2.29437600	-0.74946800
C	-3.27578800	1.92025800	-1.83714900
H	-3.58197500	0.90038100	0.02550800
C	-2.36699100	2.56146300	-2.67683700
H	-0.32046400	3.18206800	-2.90363700
H	-4.31144900	1.81081300	-2.13979800
H	-2.68527800	2.95947000	-3.63268100
Li	0.41099100	-1.20649700	3.49351600
H	-1.92116000	0.55517300	1.75438900
C	3.58030500	-0.25332900	-0.23597200
C	3.64128100	-1.64209600	-0.40939400
C	4.57364600	0.56527800	-0.78746400
C	4.68896200	-2.20250500	-1.12773700
H	2.86830400	-2.26813400	0.02043100
C	5.61657400	-0.00518700	-1.50506100

H	4.51934300	1.63800900	-0.64873900
C	5.67607400	-1.38644400	-1.67564700
H	4.73510900	-3.27637500	-1.26091700
H	6.38439700	0.62873200	-1.93122600
H	6.49191500	-1.82697100	-2.23594100
O	-0.25975300	-1.85228200	1.86082900
C	-0.58689200	-1.45361000	0.73540500
H	0.17103600	-1.07110300	0.03771600
C	-1.89689700	-1.77242300	0.12714100
C	-2.93935900	-2.28882600	0.90247000
C	-2.08280700	-1.56175700	-1.23870600
C	-4.15791900	-2.58850000	0.31091400
H	-2.77943600	-2.44694600	1.96296000
C	-3.30097600	-1.87677100	-1.83392800
H	-1.27508800	-1.14274100	-1.83095600
C	-4.33791200	-2.38617400	-1.05973900
H	-4.96959300	-2.98370700	0.91014300
H	-3.44324600	-1.71290100	-2.89536800
H	-5.28943400	-2.62561700	-1.51985500

Zero-point correction=	0.331816 (Hartree/Particle)
Thermal correction to Energy=	0.355615
Thermal correction to Enthalpy=	0.356560
Thermal correction to Gibbs Free Energy=	0.274724
Sum of electronic and zero-point Energies=	-1479.413223
Sum of electronic and thermal Energies=	-1479.389423
Sum of electronic and thermal Enthalpies=	-1479.388479
Sum of electronic and thermal Free Energies=	-1479.470314

Imaginary Frequency	-157.31 cm ⁻¹
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PC_g[‡]

S	1.47505300	-1.44630800	-1.54030700
O	1.74182300	-1.14788900	-2.95125300
O	1.53652000	-2.89421800	-1.20458200
C	-0.16790000	-0.96000400	-1.30162800
C	-1.28345600	-0.51723100	-1.18281000
C	2.38760900	-0.62428000	-0.37942000
C	2.52497300	0.82056700	-0.35920000
C	1.65246700	1.72131600	-0.99912100
C	3.54200000	1.37063400	0.44873800
C	1.77251100	3.09330900	-0.80514700
H	0.87517800	1.35553200	-1.65844000
C	3.65628000	2.74057600	0.63656800
H	4.24410300	0.70252900	0.93786400

C	2.76437900	3.61729100	0.01926700
H	1.08175800	3.75946500	-1.31043100
H	4.44772100	3.12704500	1.26902400
H	2.85055400	4.68666800	0.16781100
Li	1.45988500	-3.86779400	0.43083700
H	3.25729800	-1.23187300	-0.15240500
C	-2.59568600	0.02109000	-1.00909800
C	-3.69019000	-0.82905500	-0.81858100
C	-2.77150700	1.40953700	-0.98042200
C	-4.95002800	-0.28954800	-0.59353300
H	-3.54276600	-1.90211300	-0.83559900
C	-4.03485000	1.93934200	-0.75559800
H	-1.91455300	2.05880100	-1.11729100
C	-5.12360300	1.09229800	-0.55868100
H	-5.79688200	-0.94774500	-0.44207000
H	-4.16983900	3.01376300	-0.72892900
H	-6.10743200	1.50910600	-0.37942600
O	1.87648000	-2.60267400	1.75345200
C	1.70180800	-1.37473600	1.79401200
H	2.53557600	-0.70840900	2.05146900
C	0.35726600	-0.76533500	1.91931900
C	-0.77519200	-1.57797800	2.01157000
C	0.22359300	0.62313300	2.00389400
C	-2.03012400	-1.00843000	2.18235600
H	-0.65956600	-2.65453200	1.96131600
C	-1.03638700	1.19192400	2.15462100
H	1.10585000	1.25271700	1.94290100
C	-2.16265000	0.37727000	2.24732500
H	-2.90787400	-1.63999000	2.25606800
H	-1.14058600	2.26963500	2.20384400
H	-3.14551500	0.82181500	2.35917700

Zero-point correction= 0.332249 (Hartree/Particle)
 Thermal correction to Energy= 0.355777
 Thermal correction to Enthalpy= 0.356721
 Thermal correction to Gibbs Free Energy= 0.277567
 Sum of electronic and zero-point Energies= -1479.414145
 Sum of electronic and thermal Energies= -1479.390617
 Sum of electronic and thermal Enthalpies= -1479.389673
 Sum of electronic and thermal Free Energies= -1479.468827

Imaginary Frequency -149.58 cm⁻¹

PC_h[‡]

S	1.01958000	-1.57212600	-0.43722400
O	1.25307500	-1.18434900	-1.85972400
O	1.29669600	-3.00338100	-0.23426500
C	-0.66490400	-1.34589900	-0.12788500
C	-1.84702500	-1.22834200	0.07816700
C	1.71237000	-0.45958100	0.62502900
C	3.15229800	-0.30566100	0.68860200
C	4.05027900	-0.74638100	-0.30473900
C	3.69909500	0.40392200	1.77961700
C	5.41388600	-0.49273100	-0.20194100
H	3.68605900	-1.30901900	-1.15671200
C	5.06015400	0.65484500	1.87257200
H	3.03280800	0.75643500	2.56102000
C	5.93463400	0.21009200	0.88098600
H	6.07695400	-0.85460300	-0.98017000
H	5.44240600	1.20143700	2.72771000
H	6.99760200	0.40406100	0.95438500
Li	1.93111800	0.26206800	-2.86894600
H	1.13447000	-0.39199200	1.53998900
C	-3.24556500	-1.03919300	0.30587100
C	-3.71658600	-0.78371900	1.59868200
C	-4.13434100	-1.04957200	-0.77506800
C	-5.06673500	-0.53183100	1.80265800
H	-3.01981300	-0.76956900	2.42801600
C	-5.48330500	-0.79876900	-0.56059200
H	-3.75886600	-1.24131200	-1.77290200
C	-5.95028100	-0.53545300	0.72521100
H	-5.42998900	-0.32910100	2.80280300
H	-6.17013500	-0.80425300	-1.39816300
H	-7.00247100	-0.33521500	0.88807300
O	1.96359700	1.66548900	-1.59621100
C	1.37823100	1.81299700	-0.52506800
H	1.94654000	2.07651900	0.37719000
C	-0.09308900	1.91260200	-0.40741200
C	-0.91224100	1.82918800	-1.53412600
C	-0.66028100	2.12716900	0.85050900
C	-2.29089500	1.94380100	-1.39954500
H	-0.46502800	1.68470200	-2.51061300
C	-2.03733200	2.24135400	0.98458900
H	-0.01495900	2.18863000	1.72166200
C	-2.85351000	2.14613600	-0.14158000
H	-2.92902900	1.87111500	-2.27248400
H	-2.47830800	2.39523800	1.96232300
H	-3.93096700	2.21282800	-0.03532200

Zero-point correction=	0.332298 (Hartree/Particle)
Thermal correction to Energy=	0.355738
Thermal correction to Enthalpy=	0.356682

Thermal correction to Gibbs Free Energy=	0.278080
Sum of electronic and zero-point Energies=	-1479.411498
Sum of electronic and thermal Energies=	-1479.388059
Sum of electronic and thermal Enthalpies=	-1479.387114
Sum of electronic and thermal Free Energies=	-1479.465717

Imaginary Frequency	-83.73 cm ⁻¹
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Products of Benzaldehyde Addition to the Lithiated Sulfone:

9a

S	-0.05549000	-2.22541400	0.14840300
O	0.11989400	-2.58577200	1.56620300
O	0.13259500	-3.28824700	-0.83080700
C	-1.64671800	-1.59588000	-0.00045900
C	-2.64936600	-0.94655200	-0.16952900
C	0.97768000	-0.80370400	-0.30927800
C	0.62008900	0.40355700	0.51101400
C	0.98398500	0.52704600	1.85468400
C	-0.08771700	1.44223800	-0.09957100
C	0.64056600	1.67057700	2.56900000
H	1.55074800	-0.26617500	2.32288400
C	-0.42870600	2.58570900	0.61515800
H	-0.37348700	1.35358300	-1.14288300
C	-0.06756300	2.70025600	1.95454600
H	0.92924800	1.75842300	3.60984800
H	-0.97659000	3.38300700	0.12667200
H	-0.33341500	3.58836900	2.51571100
Li	2.01727000	-2.90211900	2.09307200
H	0.67915800	-0.64369000	-1.34973200
C	-3.83453700	-0.16998900	-0.34205400
C	-4.83026700	-0.58376000	-1.23503600
C	-3.98158600	1.02055000	0.38196600
C	-5.96905500	0.19306500	-1.39733600
H	-4.70359800	-1.50494700	-1.79002600
C	-5.12388600	1.78989000	0.20835300
H	-3.19925300	1.32950300	1.06542400
C	-6.11620500	1.37731700	-0.67828400
H	-6.74198700	-0.12462300	-2.08606900
H	-5.24063300	2.71139900	0.76513500
H	-7.00642600	1.98049000	-0.80985700
O	2.83316800	-1.82406500	0.92763200
C	2.48226800	-1.29927800	-0.26671700
H	2.53996600	-2.03113400	-1.09587900
C	3.31112200	-0.09030400	-0.70666900

C	4.04580900	0.62957600	0.23173300
C	3.32201700	0.32329500	-2.03958500
C	4.77491300	1.75260400	-0.15333600
H	4.03724500	0.28834500	1.26014700
C	4.04837300	1.44496900	-2.42869500
H	2.76417600	-0.24156100	-2.78194100
C	4.77601300	2.16539700	-1.48333300
H	5.34456900	2.30616200	0.58478900
H	4.05299700	1.75322600	-3.46797700
H	5.34467500	3.03778900	-1.78357000

Zero-point correction= 0.335610 (Hartree/Particle)
 Thermal correction to Energy= 0.358938
 Thermal correction to Enthalpy= 0.359883
 Thermal correction to Gibbs Free Energy= 0.279118
 Sum of electronic and zero-point Energies= -1479.434499
 Sum of electronic and thermal Energies= -1479.411171
 Sum of electronic and thermal Enthalpies= -1479.410227
 Sum of electronic and thermal Free Energies= -1479.490991

9b

S	0.56386500	-0.26672200	1.38636100
O	0.52862900	0.71488600	2.48454600
O	1.34183300	-1.47924900	1.59261100
C	-1.07407300	-0.71414300	1.10530500
C	-2.19369100	-0.96762100	0.73568900
C	1.02752000	0.52160700	-0.19217800
C	0.09219400	1.66488800	-0.48477600
C	0.31505200	2.93675900	0.04881700
C	-1.00749400	1.46026400	-1.32175600
C	-0.55535100	3.98102300	-0.24455800
H	1.18162800	3.09729800	0.67914900
C	-1.87847000	2.50509200	-1.61358400
H	-1.18047900	0.47778700	-1.74905300
C	-1.65624700	3.76732200	-1.07068500
H	-0.37299200	4.96493100	0.17125700
H	-2.72602400	2.33297400	-2.26668200
H	-2.33297400	4.58296100	-1.29643200
Li	2.24815600	1.68527800	2.71807700
H	0.85602000	-0.28890100	-0.90568200
C	-3.52676200	-1.23497900	0.29965100
C	-4.37445900	-0.16234200	-0.00652700
C	-3.97664800	-2.55372200	0.16226200
C	-5.66644900	-0.41445700	-0.44717300
H	-4.01114100	0.85267800	0.10220400

C	-5.27154500	-2.79277400	-0.27695500
H	-3.31131700	-3.37448900	0.39968900
C	-6.11500200	-1.72655000	-0.58165700
H	-6.32403600	0.41252200	-0.68484500
H	-5.62297400	-3.81159200	-0.38289100
H	-7.12426600	-1.91878600	-0.92521900
O	2.90378400	1.42487600	1.09266200
C	2.56162600	0.90587000	-0.10760100
H	2.65179900	1.64147300	-0.93304600
C	3.41402100	-0.29328900	-0.54437200
C	4.33291500	-0.86287900	0.33076300
C	3.30933100	-0.80518000	-1.83947200
C	5.12293400	-1.93762200	-0.07237900
H	4.41327500	-0.45005000	1.32870100
C	4.09482500	-1.87824100	-2.24774600
H	2.61244700	-0.35417300	-2.54168200
C	5.00496700	-2.45100800	-1.36084200
H	5.83280200	-2.37537900	0.62065000
H	4.00270100	-2.26364600	-3.25679900
H	5.62009500	-3.28610400	-1.67521500

Zero-point correction=	0.335568 (Hartree/Particle)
Thermal correction to Energy=	0.358864
Thermal correction to Enthalpy=	0.359808
Thermal correction to Gibbs Free Energy=	0.279074
Sum of electronic and zero-point Energies=	-1479.431282
Sum of electronic and thermal Energies=	-1479.407986
Sum of electronic and thermal Enthalpies=	-1479.407042
Sum of electronic and thermal Free Energies=	-1479.487776

9c

S	-0.39284800	-1.86900900	-0.19983300
O	-1.04118700	-1.62279000	-1.48016700
O	-0.46266700	-3.24085900	0.33461100
C	1.28293900	-1.50595200	-0.35330300
C	2.40646300	-1.06800600	-0.35792100
C	-0.91412500	-0.67026900	1.07046100
C	-0.33218600	0.69087300	0.79976500
C	-0.52163900	1.35737300	-0.41542700
C	0.40609800	1.31357900	1.80759600
C	0.02382000	2.62080000	-0.61266600
H	-1.09798300	0.88671600	-1.20397400
C	0.93545900	2.58685900	1.61621600
H	0.56583700	0.79882700	2.74923400
C	0.74780900	3.24187800	0.40307400
H	-0.12442500	3.12538600	-1.56006300

H	1.50008400	3.06025800	2.41066500
H	1.16482700	4.22996500	0.24770500
Li	-2.20308300	-3.71059000	1.16044600
H	-0.44552100	-1.10184000	1.95961700
C	3.71779000	-0.50419400	-0.37219400
C	3.84898300	0.89085100	-0.36164300
C	4.85256000	-1.32326300	-0.38612400
C	5.11596300	1.45829900	-0.36502400
H	2.95841700	1.50980200	-0.34726200
C	6.11382900	-0.74312400	-0.39229600
H	4.73726900	-2.39996500	-0.39243600
C	6.24630500	0.64376200	-0.38147200
H	5.22200700	2.53609900	-0.35582100
H	6.99451100	-1.37318800	-0.40447500
H	7.23313200	1.09072500	-0.38534300
O	-2.85888400	-2.08025100	1.38151600
C	-2.48093200	-0.78562900	1.31313300
H	-2.56789900	-0.25421500	2.28312300
C	-3.28890800	0.05383100	0.32166200
C	-3.84491400	-0.52697800	-0.81643500
C	-3.51068900	1.41049200	0.56024200
C	-4.57910700	0.24020000	-1.71633300
H	-3.69099600	-1.58507100	-0.98741500
C	-4.24660600	2.18326700	-0.33406000
H	-3.09526500	1.86924800	1.45325500
C	-4.77805300	1.59945200	-1.48097800
H	-5.00139200	-0.22240100	-2.60142300
H	-4.40825400	3.23647100	-0.13437500
H	-5.35277700	2.19567800	-2.18035200

Zero-point correction=	0.335297 (Hartree/Particle)
Thermal correction to Energy=	0.358753
Thermal correction to Enthalpy=	0.359697
Thermal correction to Gibbs Free Energy=	0.279526
Sum of electronic and zero-point Energies=	-1479.431991
Sum of electronic and thermal Energies=	-1479.408536
Sum of electronic and thermal Enthalpies=	-1479.407592
Sum of electronic and thermal Free Energies=	-1479.487763

9d

S	-0.03553200	-2.19905100	-0.45680100
O	-0.18081300	-2.40646400	-1.89215700
O	-0.25817600	-3.36238700	0.42005300
C	1.56092200	-1.64836300	-0.14097400
C	2.57905500	-1.04422800	0.08928900

C	-1.05933000	-0.79097900	0.08463700
C	-0.46398600	0.51163200	-0.36766700
C	-0.30809800	0.81054200	-1.72370000
C	-0.10080100	1.46265200	0.58726800
C	0.20143500	2.04532900	-2.11323800
H	-0.57929200	0.07576600	-2.47340500
C	0.39812800	2.70091100	0.19656900
H	-0.21931900	1.23382700	1.64111100
C	0.55096600	2.99456900	-1.15590900
H	0.32117500	2.26765000	-3.16693000
H	0.67013500	3.43336500	0.94732100
H	0.94191800	3.95750900	-1.46271400
Li	-2.18351600	-3.80758900	0.66325700
H	-1.03542400	-0.87865600	1.17488000
C	3.76877700	-0.29276300	0.32741600
C	3.82951500	1.02890600	-0.13432500
C	4.85079100	-0.85483300	1.01444700
C	4.97353400	1.78097200	0.09491600
H	2.97979300	1.44896100	-0.66129000
C	5.99032200	-0.09291700	1.23413400
H	4.79049200	-1.87694400	1.36694100
C	6.05225500	1.22159800	0.77655600
H	5.02439200	2.80327600	-0.25903800
H	6.83069500	-0.52430800	1.76366000
H	6.94370400	1.81164000	0.95208800
O	-2.91369400	-2.33150900	-0.00483800
C	-2.52526300	-1.09835100	-0.40352000
H	-2.49851300	-0.98271300	-1.50388500
C	-3.38946200	0.04012200	0.14264400
C	-3.90270200	-0.04895700	1.43590300
C	-3.66118600	1.17929100	-0.61493300
C	-4.66481100	0.98666400	1.96906000
H	-3.70744300	-0.94703200	2.01149600
C	-4.42567400	2.21720500	-0.08711000
H	-3.27175200	1.25426300	-1.62565100
C	-4.92668900	2.12481500	1.20881600
H	-5.05899000	0.90580500	2.97585400
H	-4.63401800	3.09479000	-0.68848200
H	-5.52321500	2.93037000	1.62094800

Zero-point correction=	0.335295 (Hartree/Particle)
Thermal correction to Energy=	0.358806
Thermal correction to Enthalpy=	0.359750
Thermal correction to Gibbs Free Energy=	0.279059
Sum of electronic and zero-point Energies=	-1479.437028
Sum of electronic and thermal Energies=	-1479.413517
Sum of electronic and thermal Enthalpies=	-1479.412573
Sum of electronic and thermal Free Energies=	-1479.493264

9e

S	0.19188900	-1.93244100	0.09546100
O	0.08031700	-2.96040300	-0.93070200
O	-0.08591500	-2.36081300	1.47671700
C	1.79269100	-1.31121900	0.06129800
C	2.87924600	-0.79505900	-0.02423400
C	-0.83446400	-0.50072400	-0.35667800
C	-2.27033400	-0.95883900	-0.30091500
C	-3.01239300	-0.91377700	0.88280500
C	-2.87721600	-1.42615100	-1.46888000
C	-4.34010900	-1.32701400	0.88992000
H	-2.54556400	-0.53177200	1.78110800
C	-4.20459800	-1.84214300	-1.45885800
H	-2.30583800	-1.46250200	-2.39023500
C	-4.93844400	-1.79435300	-0.27762900
H	-4.91050200	-1.28202800	1.81025000
H	-4.66379600	-2.20011000	-2.37251900
H	-5.97290500	-2.11683400	-0.26699400
Li	-0.13059100	-0.95914900	2.86124700
H	-0.54294000	-0.34354200	-1.39946800
C	4.16475400	-0.17690500	-0.09081800
C	5.16333000	-0.71159400	-0.91387200
C	4.41465200	0.97263400	0.66961600
C	6.40615000	-0.09590200	-0.97003400
H	4.95754100	-1.59969800	-1.49835100
C	5.66090200	1.58009600	0.60360000
H	3.63232200	1.37672600	1.30075600
C	6.65529800	1.04722100	-0.21371800
H	7.18093900	-0.50760500	-1.60476900
H	5.85682400	2.46930900	1.18979700
H	7.62670800	1.52430000	-0.26186300
O	-0.38196300	0.48179200	1.84215600
C	-0.42320500	0.74662700	0.51616500
H	0.56625300	1.03823600	0.11050000
C	-1.37414300	1.88012300	0.11553800
C	-2.27797200	2.39559900	1.03925900
C	-1.35039100	2.41106200	-1.17628700
C	-3.15463200	3.41732500	0.67784600
H	-2.27528700	1.98529700	2.04187800
C	-2.22504300	3.42881500	-1.54254100
H	-0.63541400	2.03235800	-1.90187800
C	-3.13432100	3.93385600	-0.61434900
H	-3.85417800	3.81150000	1.40655600
H	-2.19491200	3.83222900	-2.54828400
H	-3.81576700	4.72796300	-0.89637600

Zero-point correction=	0.335538 (Hartree/Particle)
Thermal correction to Energy=	0.358984
Thermal correction to Enthalpy=	0.359929
Thermal correction to Gibbs Free Energy=	0.278713
Sum of electronic and zero-point Energies=	-1479.433071
Sum of electronic and thermal Energies=	-1479.409625
Sum of electronic and thermal Enthalpies=	-1479.408681
Sum of electronic and thermal Free Energies=	-1479.489896

9f

S	-0.18828900	-1.36217900	1.85220400
O	-0.14058000	-0.89743900	3.24964700
O	-0.16301400	-2.80569500	1.66067700
C	-1.63472600	-0.75413000	1.15207600
C	-2.58443600	-0.29343500	0.56890400
C	1.15167100	-0.56347500	0.90897400
C	1.45265700	-1.33118400	-0.34603900
C	0.55050900	-1.36543000	-1.41278900
C	2.68508500	-1.97150800	-0.47703700
C	0.87978400	-2.03082800	-2.58868700
H	-0.41039500	-0.86963600	-1.33108900
C	3.01842000	-2.62857300	-1.65710100
H	3.39100200	-1.94517300	0.34610100
C	2.11546900	-2.66018700	-2.71552500
H	0.17224800	-2.05272100	-3.40897000
H	3.98183500	-3.11578200	-1.74840400
H	2.37266300	-3.17272900	-3.63479300
Li	0.07749500	1.04598100	3.54506200
H	1.97360300	-0.65309100	1.62895400
C	-3.70497000	0.27711400	-0.10730900
C	-3.76503800	1.66558900	-0.28353700
C	-4.72952700	-0.54334800	-0.59502500
C	-4.84920600	2.22568300	-0.94474800
H	-2.96416200	2.28759000	0.09791900
C	-5.80959700	0.02911500	-1.25269300
H	-4.67103400	-1.61542400	-0.45374400
C	-5.87006900	1.40991800	-1.42789600
H	-4.89825300	3.29860500	-1.08302900
H	-6.60460400	-0.60216500	-1.62971500
H	-6.71495400	1.85141900	-1.94251000
O	0.47511600	1.54815300	1.89020400
C	0.84443400	0.97215600	0.72496700
H	0.05909000	1.02612400	-0.05455000
C	2.11324200	1.56855700	0.10758000
C	3.16194600	1.95706800	0.94065200

C	2.25678100	1.71740700	-1.27157200
C	4.33837500	2.47404300	0.40623100
H	3.03712500	1.86103100	2.01377300
C	3.43126600	2.23695000	-1.81167100
H	1.44343600	1.42405100	-1.92822700
C	4.47708900	2.61366600	-0.97347100
H	5.14652100	2.77274700	1.06440800
H	3.52777200	2.35146500	-2.88533300
H	5.39110700	3.01943800	-1.39117500

Zero-point correction= 0.335284 (Hartree/Particle)
 Thermal correction to Energy= 0.358834
 Thermal correction to Enthalpy= 0.359779
 Thermal correction to Gibbs Free Energy= 0.277957
 Sum of electronic and zero-point Energies= -1479.434666
 Sum of electronic and thermal Energies= -1479.411116
 Sum of electronic and thermal Enthalpies= -1479.410172
 Sum of electronic and thermal Free Energies= -1479.491993

9g

S	1.49660800	-1.02095900	-1.59131900
O	2.22768400	-0.33608500	-2.64961100
O	1.36199600	-2.48080500	-1.72785100
C	-0.09743700	-0.39104900	-1.54603000
C	-1.22526000	-0.00128100	-1.37501400
C	2.27148300	-0.62447300	0.00136100
C	2.40936500	0.86984700	0.15694000
C	1.32515300	1.71963500	0.39622500
C	3.69073900	1.42361300	0.07873400
C	1.52321600	3.08805300	0.55229800
H	0.32414200	1.31802800	0.46728100
C	3.88980200	2.78972700	0.24323400
H	4.53983100	0.77648700	-0.11257100
C	2.80368600	3.62747900	0.47818300
H	0.67157500	3.73271100	0.73582800
H	4.89130000	3.19846100	0.18246500
H	2.95410100	4.69326700	0.60229300
Li	1.92359900	-3.81876800	-0.40476100
H	3.26441800	-1.04181000	-0.20517200
C	-2.55044600	0.46248500	-1.12448300
C	-3.63100700	-0.42077500	-1.23669300
C	-2.75659100	1.78534200	-0.71482700
C	-4.91105300	0.02171500	-0.93492400
H	-3.45583400	-1.44259500	-1.55014500
C	-4.04104700	2.21522700	-0.41038900
H	-1.91280700	2.46037500	-0.63479800

C	-5.11598200	1.33570500	-0.51841800
H	-5.74911900	-0.65892100	-1.02003500
H	-4.20389300	3.23658600	-0.08941600
H	-6.11655800	1.67563700	-0.27970200
O	2.08061900	-2.79966200	1.04620100
C	1.77693100	-1.49653000	1.23777600
H	2.37212500	-1.02942800	2.04816400
C	0.31111600	-1.25282500	1.61451200
C	-0.69336300	-2.08465500	1.11771700
C	-0.04709700	-0.23316000	2.49679900
C	-2.02611400	-1.87430700	1.45494300
H	-0.42150300	-2.90076100	0.45831300
C	-1.38125700	-0.01282100	2.83516600
H	0.72640100	0.40024900	2.92058500
C	-2.37691700	-0.82970600	2.30784200
H	-2.79470700	-2.52432400	1.05150200
H	-1.63971600	0.78877500	3.51780700
H	-3.41619000	-0.66213300	2.56735700

Zero-point correction=	0.336051 (Hartree/Particle)
Thermal correction to Energy=	0.359062
Thermal correction to Enthalpy=	0.360006
Thermal correction to Gibbs Free Energy=	0.282037
Sum of electronic and zero-point Energies=	-1479.429848
Sum of electronic and thermal Energies=	-1479.406838
Sum of electronic and thermal Enthalpies=	-1479.405894
Sum of electronic and thermal Free Energies=	-1479.483862

9h

S	-1.23556200	-1.54830700	0.04262300
O	-1.72510900	-1.98264300	1.36126100
O	-1.67772700	-2.34670600	-1.09447100
C	0.47473400	-1.57748600	0.07120600
C	1.66297200	-1.39989500	-0.03720500
C	-1.65305400	0.19863300	-0.27900700
C	-3.16258000	0.25725400	-0.34036000
C	-3.91745200	0.62078100	0.77788000
C	-3.81571500	-0.04191200	-1.53848500
C	-5.30455700	0.68423600	0.69302800
H	-3.40685100	0.86180200	1.70309400
C	-5.20264500	0.01925200	-1.61998700
H	-3.23284700	-0.32427000	-2.40818000
C	-5.95011400	0.38115000	-0.50285300
H	-5.88255400	0.97254600	1.56312700
H	-5.69769400	-0.21142500	-2.55568800
H	-7.03077000	0.43095800	-0.56516100

Li	-1.53404200	-0.75999700	2.88562800
H	-1.24388600	0.33181900	-1.28372600
C	3.06532600	-1.16901800	-0.14939700
C	3.61721000	-0.86990700	-1.40021200
C	3.87173900	-1.18622100	0.99494600
C	4.97166400	-0.58323600	-1.50006800
H	2.97969300	-0.85149900	-2.27562300
C	5.22500500	-0.90190700	0.88290700
H	3.42880100	-1.40911200	1.95798100
C	5.77391600	-0.59672000	-0.36135900
H	5.40109200	-0.34519100	-2.46541300
H	5.85171100	-0.91136400	1.76612900
H	6.83019400	-0.36992600	-0.44336600
O	-1.05492200	0.71870000	2.03516900
C	-0.99796100	1.18120900	0.76483400
H	-1.61827000	2.09118800	0.61971400
C	0.41085100	1.61346100	0.32297800
C	1.45386600	1.59401600	1.24488700
C	0.66358600	2.10456300	-0.96120300
C	2.72657000	2.04008200	0.89299000
H	1.24631900	1.21591200	2.23857600
C	1.93521400	2.54155600	-1.32048100
H	-0.13893200	2.16438400	-1.69104600
C	2.97458800	2.51016000	-0.39223900
H	3.52895200	2.00955000	1.62218900
H	2.11329000	2.91357700	-2.32325800
H	3.96596000	2.84882400	-0.67067200

Zero-point correction= 0.335565 (Hartree/Particle)
 Thermal correction to Energy= 0.358754
 Thermal correction to Enthalpy= 0.359698
 Thermal correction to Gibbs Free Energy= 0.281090
 Sum of electronic and zero-point Energies= -1479.433718
 Sum of electronic and thermal Energies= -1479.410529
 Sum of electronic and thermal Enthalpies= -1479.409585
 Sum of electronic and thermal Free Energies= -1479.488193

Cyclization to Form Oxathiin Ring:

9_{cis}

S	-0.19222300	-1.93205000	-0.09581800
O	0.08543400	-2.36051500	-1.47707400

O	-0.08090700	-2.96004000	0.93034600
C	-1.79288800	-1.31047600	-0.06163400
C	-2.87949500	-0.79445100	0.02405500
C	0.83447000	-0.50058900	0.35639100
C	0.42373700	0.74684200	-0.51656500
H	-0.56578200	1.03867000	-0.11120400
O	0.38285400	0.48203000	-1.84257300
C	2.27024000	-0.95906300	0.30093000
C	3.01260000	-0.91412700	-0.88260600
C	2.87674500	-1.42652900	1.46903300
C	4.34023200	-1.32764500	-0.88940600
H	2.54609300	-0.53197500	-1.78101400
C	4.20404000	-1.84279900	1.45932400
H	2.30513800	-1.46277100	2.39025000
C	4.93818600	-1.79513700	0.27827400
H	4.91086000	-1.28274700	-1.80959500
H	4.66294100	-2.20087700	2.37309100
H	5.97258300	-2.11783000	0.26788600
C	1.37480300	1.88014100	-0.11567300
C	1.35092200	2.41101200	1.17617800
C	2.27886000	2.39552700	-1.03922000
C	2.22566200	3.42862100	1.54262200
H	0.63576800	2.03238500	1.90163500
C	3.15561200	3.41710800	-0.67761500
H	2.27626600	1.98526500	-2.04185500
C	3.13516400	3.93357700	0.61460200
H	2.19542700	3.83199100	2.54837900
H	3.85533300	3.81121700	-1.40619100
H	3.81667700	4.72757300	0.89677900
C	-4.16511800	-0.17655200	0.09081800
C	-4.41554100	0.97266900	-0.66992100
C	-5.16331000	-0.71122400	0.91435000
C	-5.66192900	1.57983000	-0.60373100
H	-3.63351100	1.37675300	-1.30143600
C	-6.40627300	-0.09583700	0.97068200
H	-4.95711700	-1.59908400	1.49905800
C	-6.65594300	1.04697000	0.21406000
H	-5.85826000	2.46879400	-1.19016800
H	-7.18076500	-0.50753200	1.60578400
H	-7.62746400	1.52381100	0.26233300
Li	0.13163600	-0.95885200	-2.86167900
H	0.54278900	-0.34329000	1.39912000

Zero-point correction=	0.335535 (Hartree/Particle)
Thermal correction to Energy=	0.358984
Thermal correction to Enthalpy=	0.359928
Thermal correction to Gibbs Free Energy=	0.278693
Sum of electronic and zero-point Energies=	-1479.433074

Sum of electronic and thermal Energies=	-1479.409625
Sum of electronic and thermal Enthalpies=	-1479.408681
Sum of electronic and thermal Free Energies=	-1479.489916

9_{trans}

S	0.19127900	1.34830300	1.85728800
O	0.14918500	0.87439500	3.25175500
O	0.16682000	2.79304900	1.67509000
C	1.63478000	0.74332400	1.14828500
C	2.58663400	0.28686300	0.56535000
C	-1.15290600	0.55771200	0.91362200
C	-0.85066800	-0.97785800	0.72183500
H	-0.06504100	-1.03037500	-0.05750500
O	-0.48415400	-1.56114700	1.88426100
C	-1.45441500	1.33162200	-0.33750400
C	-0.55452900	1.36756800	-1.40610200
C	-2.68543300	1.97568300	-0.46340900
C	-0.88453300	2.03843200	-2.57868800
H	0.40517000	0.86882100	-1.32850700
C	-3.01958000	2.63811800	-1.64021200
H	-3.38977100	1.94784800	0.36103000
C	-2.11881200	2.67150700	-2.70045600
H	-0.17868400	2.06161700	-3.40038900
H	-3.98196900	3.12806700	-1.72759700
H	-2.37663000	3.18822900	-3.61720700
C	-2.12084100	-1.56705700	0.10059700
C	-2.26064900	-1.71563000	-1.27888800
C	-3.17439200	-1.94946100	0.93041100
C	-3.43597800	-2.22950300	-1.82263300
H	-1.44366500	-1.42657800	-1.93294200
C	-4.35167300	-2.46062000	0.39239500
H	-3.05286200	-1.85331500	2.00391300
C	-4.48643800	-2.60045600	-0.98771500
H	-3.52950600	-2.34409100	-2.89655100
H	-5.16361000	-2.75461100	1.04801700
H	-5.40110700	-3.00184700	-1.40821700
C	3.71029700	-0.27702700	-0.11132300
C	4.73035400	0.54990300	-0.59751700
C	3.77867600	-1.66491000	-0.28891100
C	5.81416200	-0.01547200	-1.25514800
H	4.66549000	1.62144600	-0.45506600
C	4.86655100	-2.21792100	-0.95003900
H	2.98135700	-2.29210200	0.09144500
C	5.88287100	-1.39569200	-1.43174500
H	6.60564900	0.62088500	-1.63101900
H	4.92201700	-3.29038200	-1.08935700
H	6.73063100	-1.83169600	-1.94631400

Li	-0.06350800	-1.07210000	3.53728800
H	-1.97306700	0.64641100	1.63572600

Zero-point correction=	0.335206 (Hartree/Particle)
Thermal correction to Energy=	0.358807
Thermal correction to Enthalpy=	0.359751
Thermal correction to Gibbs Free Energy=	0.277355
Sum of electronic and zero-point Energies=	-1479.434745
Sum of electronic and thermal Energies=	-1479.411143
Sum of electronic and thermal Enthalpies=	-1479.410199
Sum of electronic and thermal Free Energies=	-1479.492595

9_{cis}⁺

S	0.08250300	-2.30673300	0.22718900
O	0.21629900	-2.41247600	-1.24732300
O	0.65456900	-3.41229500	0.98991700
C	-1.58123500	-2.08007500	0.57483300
C	-2.22532700	-1.08309000	0.18177300
C	0.90395000	-0.75034700	0.76045400
C	-0.03106900	0.46643700	0.41139100
H	-0.68674600	0.56332600	1.29457600
O	-0.78949500	0.24358300	-0.71901700
C	2.29047900	-0.78406400	0.17187300
C	2.56409000	-0.24530500	-1.08813400
C	3.32434300	-1.38295400	0.89295100
C	3.84880400	-0.30403300	-1.61398600
H	1.77650100	0.24884200	-1.64357400
C	4.61187200	-1.44137100	0.36765800
H	3.11800200	-1.80420700	1.87093200
C	4.87591600	-0.90314200	-0.88757700
H	4.05065800	0.12326900	-2.58901400
H	5.40649800	-1.90440800	0.94028400
H	5.87819900	-0.94420000	-1.29719300
C	0.75886700	1.77126600	0.36900200
C	1.61168800	2.12290300	1.41865900
C	0.60409300	2.64992900	-0.69845100
C	2.30812600	3.32528900	1.39172700
H	1.73834300	1.45138700	2.26296800
C	1.30110300	3.85741100	-0.72796400
H	-0.06479700	2.37189000	-1.50405700
C	2.15710300	4.19730800	0.31381900
H	2.96975000	3.58358400	2.21046800
H	1.17407100	4.53216100	-1.56700000
H	2.70095000	5.13430000	0.29119300
C	-3.44306500	-0.32754300	0.02868000
C	-3.46847100	1.06315700	-0.11942200

C	-4.64593200	-1.04789000	0.09143100
C	-4.68930000	1.72164900	-0.19862700
H	-2.53109000	1.59732500	-0.18879500
C	-5.85859100	-0.37779700	0.00912800
H	-4.61582900	-2.12436300	0.20770700
C	-5.88302600	1.00738700	-0.13569200
H	-4.70783800	2.79870800	-0.31309000
H	-6.78427600	-0.93826300	0.05590800
H	-6.83085200	1.52800500	-0.20188500
Li	-0.51166400	-0.83602300	-2.19251400
H	0.96590400	-0.88280700	1.84333200

Zero-point correction= 0.335365 (Hartree/Particle)
 Thermal correction to Energy= 0.357550
 Thermal correction to Enthalpy= 0.358494
 Thermal correction to Gibbs Free Energy= 0.282190
 Sum of electronic and zero-point Energies= -1479.408970
 Sum of electronic and thermal Energies= -1479.386784
 Sum of electronic and thermal Enthalpies= -1479.385840
 Sum of electronic and thermal Free Energies= -1479.462144

Imaginary Frequency -349.12 cm⁻¹

9_{trans}[‡]

S	-0.00793400	-1.87535800	1.46915200
O	-0.35549800	-1.37817800	2.82593800
O	0.66437000	-3.16950900	1.43069900
C	-1.44181700	-1.87601600	0.52574800
C	-2.08674100	-0.83830300	0.26128300
C	1.06204100	-0.58554800	0.73229800
C	0.18854300	0.63111300	0.24980600
H	-0.08999600	0.40575600	-0.79410600
O	-0.93029500	0.81314400	1.02982000
C	1.97420600	-1.14607500	-0.31876000
C	1.45932500	-1.66748000	-1.50913200
C	3.35532200	-1.10500500	-0.13431900
C	2.31559600	-2.13956700	-2.49651100
H	0.38515200	-1.71155300	-1.66171700
C	4.21386300	-1.56735000	-1.12783600
H	3.76018500	-0.69913300	0.78657200
C	3.69554900	-2.08567100	-2.31011200
H	1.90661200	-2.54738400	-3.41317300
H	5.28578300	-1.52359000	-0.97633700
H	4.36221400	-2.44854700	-3.08328100
C	1.11088300	1.84331100	0.20429100

C	1.89299400	2.09934900	-0.92326700
C	1.20850500	2.69556800	1.30303400
C	2.76423000	3.18510800	-0.94912700
H	1.81873200	1.44353700	-1.78569700
C	2.07683800	3.78352200	1.27949000
H	0.58929800	2.50797100	2.17269400
C	2.85884100	4.03002700	0.15364400
H	3.36418800	3.37444800	-1.83172600
H	2.14113400	4.44166500	2.13844600
H	3.53340300	4.87789900	0.13382400
C	-3.21826500	-0.14372900	-0.29936800
C	-4.41103100	-0.87176900	-0.42565000
C	-3.15402100	1.17631400	-0.75748900
C	-5.52400600	-0.28089800	-1.00835900
H	-4.45100300	-1.89343300	-0.06819200
C	-4.27379200	1.75518700	-1.34074800
H	-2.23494600	1.72987100	-0.62819300
C	-5.45771800	1.03235100	-1.46709100
H	-6.44355300	-0.84569300	-1.10120400
H	-4.22265000	2.77759300	-1.69504500
H	-6.32810300	1.49247500	-1.91937200
Li	-1.18828200	0.41195000	2.81976900
H	1.63062800	-0.28230200	1.61815300

Zero-point correction= 0.335417 (Hartree/Particle)
 Thermal correction to Energy= 0.357572
 Thermal correction to Enthalpy= 0.358516
 Thermal correction to Gibbs Free Energy= 0.282148
 Sum of electronic and zero-point Energies= -1479.413202
 Sum of electronic and thermal Energies= -1479.391047
 Sum of electronic and thermal Enthalpies= -1479.390102
 Sum of electronic and thermal Free Energies= -1479.466471

Imaginary Frequency -344.85 cm⁻¹

10_{cis}

S	0.02765600	-2.23717500	0.23857200
O	0.32940000	-1.96813700	1.68556700
O	0.58398700	-3.49733200	-0.26072700
C	-1.67086300	-2.07870000	-0.06170400
C	-1.99952900	-0.78512800	0.09642700
C	0.83598100	-0.88093900	-0.71526500
C	-0.05479900	0.40083800	-0.54825600
H	-0.59479800	0.52002600	-1.49319900
O	-1.05039300	0.21213100	0.46655900
C	2.30018700	-0.82979900	-0.37642300

C	2.77720800	-0.30608700	0.82913200
C	3.21550300	-1.34184500	-1.29767200
C	4.14041700	-0.28799800	1.09732300
H	2.08808500	0.09765300	1.55953000
C	4.58111300	-1.32369100	-1.03040500
H	2.85538400	-1.75379000	-2.23434400
C	5.04695700	-0.79399100	0.16799000
H	4.49682300	0.12458900	2.03370000
H	5.27732400	-1.72124000	-1.75912500
H	6.10961300	-0.77444300	0.37862700
C	0.69888200	1.68347700	-0.28608100
C	1.67145200	2.08252700	-1.20669800
C	0.43705000	2.48766900	0.81913600
C	2.39063700	3.25308500	-1.00963200
H	1.87407300	1.46645100	-2.07716300
C	1.16400600	3.66127600	1.01957100
H	-0.33863500	2.21130100	1.52199700
C	2.14450600	4.04350800	0.11256700
H	3.14456600	3.54904100	-1.72927400
H	0.95598200	4.27715400	1.88660300
H	2.70861100	4.95481700	0.27089100
C	-3.35792400	-0.21628700	-0.05098900
C	-3.57125600	1.16550600	-0.01763800
C	-4.45553500	-1.06709900	-0.23647700
C	-4.85456900	1.68498300	-0.17177400
H	-2.73115000	1.83327000	0.12772200
C	-5.73232100	-0.54630300	-0.38627200
H	-4.28732100	-2.13691400	-0.26091600
C	-5.93812200	0.83364300	-0.35472500
H	-5.00469500	2.75796100	-0.14664800
H	-6.57250600	-1.21618200	-0.52690600
H	-6.93649400	1.23819200	-0.47143100
Li	-0.57845500	-0.46715000	2.45331700
H	0.73018800	-1.23679300	-1.74117000

Zero-point correction=	0.338355 (Hartree/Particle)
Thermal correction to Energy=	0.360199
Thermal correction to Enthalpy=	0.361143
Thermal correction to Gibbs Free Energy=	0.286731
Sum of electronic and zero-point Energies=	-1479.444323
Sum of electronic and thermal Energies=	-1479.422479
Sum of electronic and thermal Enthalpies=	-1479.421535
Sum of electronic and thermal Free Energies=	-1479.495948

10_{trans}

S	0.17723500	-1.87567700	1.40215900
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O	-0.06735400	-1.42355800	2.81689200
O	0.94680400	-3.11685200	1.29386600
C	-1.33237200	-1.94580900	0.55881800
C	-1.78342200	-0.69307400	0.37370200
C	1.18722500	-0.48712800	0.69848100
C	0.19449300	0.53089600	0.08681800
H	0.00823700	0.25000300	-0.95493100
O	-1.06040700	0.46443300	0.77794000
C	2.23882800	-0.95519300	-0.26190300
C	1.88627100	-1.61672500	-1.44153200
C	3.58437400	-0.70980700	0.00662600
C	2.86672000	-2.01963300	-2.33918500
H	0.84208500	-1.83172400	-1.65072300
C	4.56716600	-1.10777600	-0.89593400
H	3.86325000	-0.19720800	0.92095600
C	4.20993900	-1.76151800	-2.07033200
H	2.58413700	-2.53734300	-3.24791300
H	5.60963000	-0.90700700	-0.67961200
H	4.97336500	-2.07342400	-2.77298200
C	0.74686000	1.93531200	0.12245800
C	1.73572100	2.28874600	-0.79940000
C	0.31605700	2.87550700	1.05624900
C	2.29594600	3.56086000	-0.77659500
H	2.06269300	1.56725500	-1.54119700
C	0.87517200	4.15155700	1.07373100
H	-0.46838300	2.62582200	1.75918200
C	1.86826600	4.49588200	0.16293800
H	3.05994800	3.82442300	-1.49824100
H	0.52882300	4.87785700	1.79951000
H	2.30071400	5.48911500	0.17812700
C	-3.06787700	-0.33571600	-0.27058100
C	-4.00707500	-1.33503300	-0.55726800
C	-3.36164300	0.98757600	-0.61504800
C	-5.20651400	-1.01724200	-1.17731700
H	-3.77753100	-2.35842700	-0.28631800
C	-4.56557900	1.30236400	-1.24110800
H	-2.64437700	1.76862900	-0.39533800
C	-5.49106600	0.30424900	-1.52382800
H	-5.92447000	-1.80027200	-1.39151900
H	-4.77821900	2.33123900	-1.50704100
H	-6.42824300	0.55048300	-2.00877000
Li	-1.12939200	0.13617900	3.03976000
H	1.64347500	-0.05908100	1.59465400

Zero-point correction=	0.337755 (Hartree/Particle)
Thermal correction to Energy=	0.359876
Thermal correction to Enthalpy=	0.360820
Thermal correction to Gibbs Free Energy=	0.284540

Sum of electronic and zero-point Energies=	-1479.447633
Sum of electronic and thermal Energies=	-1479.425513
Sum of electronic and thermal Enthalpies=	-1479.424568
Sum of electronic and thermal Free Energies=	-1479.500849

10cis'

S	0.02765600	-2.23717500	0.23857200
O	0.32940000	-1.96813700	1.68556700
O	0.58398700	-3.49733200	-0.26072700
C	-1.67086300	-2.07870000	-0.06170400
C	-1.99952900	-0.78512800	0.09642700
C	0.83598100	-0.88093900	-0.71526500
C	-0.05479900	0.40083800	-0.54825600
H	-0.59479800	0.52002600	-1.49319900
O	-1.05039300	0.21213100	0.46655900
C	2.30018700	-0.82979900	-0.37642300
C	2.77720800	-0.30608700	0.82913200
C	3.21550300	-1.34184500	-1.29767200
C	4.14041700	-0.28799800	1.09732300
H	2.08808500	0.09765300	1.55953000
C	4.58111300	-1.32369100	-1.03040500
H	2.85538400	-1.75379000	-2.23434400
C	5.04695700	-0.79399100	0.16799000
H	4.49682300	0.12458900	2.03370000
H	5.27732400	-1.72124000	-1.75912500
H	6.10961300	-0.77444300	0.37862700
C	0.69888200	1.68347700	-0.28608100
C	1.67145200	2.08252700	-1.20669800
C	0.43705000	2.48766900	0.81913600
C	2.39063700	3.25308500	-1.00963200
H	1.87407300	1.46645100	-2.07716300
C	1.16400600	3.66127600	1.01957100
H	-0.33863500	2.21130100	1.52199700
C	2.14450600	4.04350800	0.11256700
H	3.14456600	3.54904100	-1.72927400
H	0.95598200	4.27715400	1.88660300
H	2.70861100	4.95481700	0.27089100
C	-3.35792400	-0.21628700	-0.05098900
C	-3.57125600	1.16550600	-0.01763800
C	-4.45553500	-1.06709900	-0.23647700
C	-4.85456900	1.68498300	-0.17177400
H	-2.73115000	1.83327000	0.12772200
C	-5.73232100	-0.54630300	-0.38627200
H	-4.28732100	-2.13691400	-0.26091600
C	-5.93812200	0.83364300	-0.35472500
H	-5.00469500	2.75796100	-0.14664800

H	-6.57250600	-1.21618200	-0.52690600
H	-6.93649400	1.23819200	-0.47143100
Li	-1.16772488	-2.07302296	2.87477630
H	0.73018800	-1.23679300	-1.74117000

Zero-point correction=	0.338057 (Hartree/Particle)
Thermal correction to Energy=	0.360279
Thermal correction to Enthalpy=	0.361223
Thermal correction to Gibbs Free Energy=	0.284479
Sum of electronic and zero-point Energies=	-1479.462155
Sum of electronic and thermal Energies=	-1479.439934
Sum of electronic and thermal Enthalpies=	-1479.438990
Sum of electronic and thermal Free Energies=	-1479.515733

10_{trans'}

S	-0.03881500	-2.19964800	-0.10576200
O	0.51107800	-2.68842500	-1.38048300
O	0.08193500	-3.16486300	1.03310300
C	0.85201700	-0.68390600	0.35905800
H	0.54871000	-0.49733500	1.39275200
C	0.23692500	0.40813800	-0.54045300
H	0.33559600	0.10579300	-1.59059400
C	-1.69575400	-1.80382800	-0.16866000
C	-1.99560000	-0.49131000	-0.18551000
O	-1.14302900	0.58939900	-0.24662600
C	2.34312200	-0.82815700	0.26183000
C	3.10855600	-0.77851200	1.42742200
C	2.98553700	-0.98302000	-0.97043200
C	4.49539200	-0.87850600	1.36763600
H	2.61593200	-0.65418800	2.38580800
C	4.37075800	-1.08207100	-1.02855200
H	2.40257000	-1.04139300	-1.88151100
C	5.12935100	-1.02917200	0.13867900
H	5.07788700	-0.83550500	2.28015000
H	4.85950800	-1.20157100	-1.98818600
H	6.20903300	-1.10526600	0.08909000
C	0.91705500	1.73672700	-0.31632700
C	1.81273900	2.24230100	-1.25470300
C	0.68184300	2.44430300	0.86315600
C	2.47657600	3.44282900	-1.01459300
H	1.99365100	1.69725500	-2.17491900
C	1.34080300	3.64519000	1.10090500
H	-0.02523700	2.05696000	1.58871200
C	2.24244200	4.14489600	0.16334600
H	3.17176900	3.83008900	-1.74986300
H	1.15138900	4.19187700	2.01708000

H	2.75647300	5.08038600	0.34950300
C	-3.40042200	0.00004300	-0.08952900
C	-3.68066400	1.35229700	0.13072300
C	-4.46687700	-0.89799000	-0.21151400
C	-4.99773900	1.79180900	0.23853600
H	-2.86618100	2.05888500	0.22120700
C	-5.77903200	-0.45668700	-0.10984700
H	-4.25047300	-1.94319100	-0.39433000
C	-6.05080500	0.89170000	0.11900300
H	-5.19844900	2.84209300	0.41486100
H	-6.59324700	-1.16448400	-0.21290300
H	-7.07522100	1.23568200	0.19917500
Li	-1.88330000	-3.49101900	1.27238700

Zero-point correction= 0.337869 (Hartree/Particle)
 Thermal correction to Energy= 0.360210
 Thermal correction to Enthalpy= 0.361154
 Thermal correction to Gibbs Free Energy= 0.284093
 Sum of electronic and zero-point Energies= -1479.461896
 Sum of electronic and thermal Energies= -1479.439556
 Sum of electronic and thermal Enthalpies= -1479.438612
 Sum of electronic and thermal Free Energies= -1479.515673

Neutral Oxathiins:

Trans-diaryl oxathiin (5a or 5_{trans})

S	0.03414300	-2.26826000	-0.15255700
O	0.20006300	-3.27695200	0.89439800
O	0.50414600	-2.61917500	-1.49426100
C	-1.63705200	-1.76563600	-0.20550600
H	-2.34684900	-2.57755900	-0.27419400
C	-2.01751700	-0.47908600	-0.10675500
C	0.82550100	-0.71950500	0.37015100
C	0.18707900	0.41181700	-0.45413200
H	0.21658100	0.15785400	-1.51995400
O	-1.18778700	0.57997200	-0.07669100
C	2.32012700	-0.83942500	0.24883900
C	3.08932100	-0.90514200	1.41009800
C	2.95060400	-0.86981300	-0.99793600
C	4.47554700	-0.99547600	1.33046700
H	2.60194600	-0.88064400	2.37866500
C	4.33520500	-0.95979200	-1.07477600
H	2.36210000	-0.83838700	-1.90703000
C	5.09991000	-1.02171700	0.08786700
H	5.06450300	-1.04371300	2.23829500

H	4.81775800	-0.98288700	-2.04437500
H	6.17924100	-1.09073300	0.02389000
C	0.87490200	1.72986900	-0.20867100
C	0.76253500	2.34998200	1.03613200
C	1.65408600	2.31206600	-1.20421200
C	1.42834600	3.54516600	1.28045400
H	0.14611700	1.90314000	1.80866200
C	2.32541900	3.50667500	-0.95673200
H	1.73860200	1.83294900	-2.17368400
C	2.21385300	4.12317700	0.28507000
H	1.33529900	4.02597400	2.24679600
H	2.93072300	3.95515600	-1.73517700
H	2.73399400	5.05393900	0.47740900
C	-3.43931300	-0.07621100	-0.01886100
C	-3.83501500	1.16705900	-0.51941800
C	-4.38888500	-0.92588000	0.55483100
C	-5.17189700	1.54342100	-0.46698300
H	-3.09649600	1.82761700	-0.95548400
C	-5.72295200	-0.54299300	0.60828000
H	-4.08328700	-1.87369600	0.98170100
C	-6.11744500	0.68987400	0.09439200
H	-5.47498600	2.50428000	-0.86467900
H	-6.45278600	-1.20299500	1.06086100
H	-7.15842600	0.98683900	0.13811000
H	0.53415300	-0.60631100	1.41792600

Zero-point correction=	0.348663
(Hartree/Particle)	
Thermal correction to Energy=	0.369766
Thermal correction to Enthalpy=	0.370710
Thermal correction to Gibbs Free Energy=	0.296036
Sum of electronic and zero-point Energies=	-1472.467229
Sum of electronic and thermal Energies=	-1472.446126
Sum of electronic and thermal Enthalpies=	-1472.445182
Sum of electronic and thermal Free Energies=	-1472.519855

Cis-diaryl oxathiin (5_{cis})

S	-0.34510100	-1.48036400	1.17452800
O	-0.59938300	-2.90817300	1.37303500
O	-0.86428700	-0.57134400	2.19743900
C	1.36312700	-1.22859000	0.94849100
C	1.87102800	-0.54254300	-0.09191900
C	-0.94869900	-1.01820800	-0.46758500
C	-0.25080200	0.25782200	-0.98697100

H	-0.54844700	0.32294200	-2.03477900
O	1.17347800	0.07714200	-1.05851700
C	-2.45596600	-0.98644500	-0.51898700
C	-3.10141600	-1.80836800	-1.44495400
C	-3.21808600	-0.15767300	0.31096900
C	-4.48795200	-1.79741400	-1.55343100
H	-2.51552900	-2.45818100	-2.08588900
C	-4.60464500	-0.15540800	0.20442900
H	-2.73075900	0.47554900	1.04085700
C	-5.24190500	-0.96985100	-0.72759600
H	-4.97578200	-2.43767000	-2.27831900
H	-5.18831200	0.48676400	0.85301800
H	-6.32243700	-0.96160700	-0.80724500
C	-0.60135900	1.57612000	-0.33034000
C	-1.62791400	2.33600500	-0.89181800
C	0.07286000	2.06101600	0.79027700
C	-1.99885200	3.55118200	-0.32615500
H	-2.14462800	1.97080800	-1.77357500
C	-0.29070800	3.28145100	1.34962400
H	0.87865600	1.49256300	1.23881300
C	-1.33075700	4.02504500	0.79864000
H	-2.80076500	4.12921200	-0.76933400
H	0.23903700	3.64990900	2.21978400
H	-1.61271800	4.97385800	1.23929200
C	3.33073200	-0.37901000	-0.28329400
C	3.81635100	0.79213300	-0.87088200
C	4.22376500	-1.37149300	0.12770400
C	5.18548000	0.97487300	-1.02521200
H	3.12023600	1.55625100	-1.19364000
C	5.59085700	-1.18610200	-0.03495200
H	3.85095700	-2.29689800	0.55049200
C	6.07400600	-0.01202300	-0.60751900
H	5.55825300	1.88842600	-1.47214400
H	6.27864300	-1.96249800	0.27689000
H	7.14066000	0.12996900	-0.73331600
H	1.98937600	-1.66369200	1.71433400
H	-0.58815600	-1.84600200	-1.08446600

Zero-point correction=	0.349052
(Hartree/Particle)	
Thermal correction to Energy=	0.369982
Thermal correction to Enthalpy=	0.370926
Thermal correction to Gibbs Free Energy=	0.297307
Sum of electronic and zero-point Energies=	-1472.460919
Sum of electronic and thermal Energies=	-1472.439990
Sum of electronic and thermal Enthalpies=	-1472.439046
Sum of electronic and thermal Free Energies=	-1472.512665

Anionic Oxathiin Prior to Ring Opening:

11a

S	-0.70999500	-0.86877000	1.33398300
O	-1.13159700	-2.25135200	1.76538500
O	-1.03190500	-0.00460500	2.53794600
C	1.02238300	-0.83268500	1.13068400
C	1.62795400	-0.61226600	-0.05339200
C	-1.24382900	-0.47969200	-0.19273200
C	-0.31150500	0.42848800	-0.93196600
H	-0.69634000	0.54410500	-1.94475100
O	0.99820500	-0.15754800	-1.14445200
C	-2.61302700	-0.73989800	-0.61239200
C	-2.95194200	-0.79093100	-1.98043700
C	-3.66196500	-0.94674400	0.30752800
C	-4.25366500	-1.03629500	-2.39732400
H	-2.18152400	-0.66291500	-2.73221000
C	-4.95781500	-1.21512900	-0.11606900
H	-3.46277800	-0.88011800	1.37121800
C	-5.27161900	-1.25784800	-1.47196000
H	-4.47035600	-1.06874800	-3.45944200
H	-5.73400200	-1.37216500	0.62493700
H	-6.28468200	-1.45488300	-1.80027400
C	-0.14400700	1.83547200	-0.34700400
C	-1.26754300	2.46995600	0.18574500
C	1.06707300	2.52478300	-0.38437900
C	-1.18370800	3.77177900	0.66659800
H	-2.20861500	1.93252600	0.23298800
C	1.15621000	3.82286700	0.11437600
H	1.94971600	2.05199400	-0.79747400
C	0.03164100	4.45181200	0.63760500
H	-2.06547400	4.25184400	1.07476900
H	2.10774500	4.34121200	0.09094200
H	0.10091700	5.46246700	1.02222400
C	3.07658300	-0.83239000	-0.27141100
C	3.72273700	-0.18575900	-1.32909600
C	3.80992700	-1.68674100	0.55841500
C	5.08500900	-0.37171700	-1.53692600
H	3.15518000	0.45830800	-1.98861500
C	5.17045800	-1.86779100	0.34958800
H	3.31538500	-2.22967200	1.35457200
C	5.81265600	-1.20766700	-0.69599700
H	5.57704700	0.13726200	-2.35683900
H	5.72840700	-2.53431400	0.99594700
H	6.87391400	-1.35275600	-0.85870700
H	1.56524400	-1.11813200	2.02023900

Li	-1.63984000	-1.58243000	3.58633000
Zero-point correction=		0.337219	(Hartree/Particle)
Thermal correction to Energy=		0.359400	
Thermal correction to Enthalpy=		0.360345	
Thermal correction to Gibbs Free Energy=		0.284057	
Sum of electronic and zero-point Energies=		-1479.460587	
Sum of electronic and thermal Energies=		-1479.438405	
Sum of electronic and thermal Enthalpies=		-1479.437461	
Sum of electronic and thermal Free Energies=		-1479.513749	

11b

S	0.94360500	-0.29168200	1.58313800
O	1.73087900	0.70216100	2.38309800
O	0.81189300	-1.57956100	2.28227200
C	-0.66297700	0.39956900	1.41539700
C	-1.22094500	0.61919700	0.20668500
C	1.49978400	-0.36649600	-0.01959200
C	0.38485600	-0.76959700	-0.92169400
H	0.75721900	-0.73229000	-1.94718600
O	-0.72901700	0.19221400	-0.96484900
C	2.48408700	0.61331600	-0.46980800
C	2.26740400	1.42068000	-1.60667600
C	3.73022100	0.76039600	0.18054000
C	3.23447300	2.31066900	-2.06157300
H	1.31929800	1.36427300	-2.12954300
C	4.68096700	1.67562300	-0.25990100
H	3.96236700	0.11012900	1.01724000
C	4.44481100	2.45887800	-1.38860800
H	3.02872200	2.91032400	-2.94161700
H	5.62694500	1.75281100	0.26540700
H	5.19166100	3.15955900	-1.74118600
C	-0.18141800	-2.17001400	-0.69516500
C	0.71633000	-3.23815700	-0.63373800
C	-1.54592900	-2.43114900	-0.60126400
C	0.25989100	-4.54035600	-0.47919600
H	1.77927500	-3.03304300	-0.69085000
C	-2.00511800	-3.73728400	-0.43032900
H	-2.26399700	-1.62225500	-0.65504300
C	-1.10662000	-4.79512900	-0.37011100
H	0.97040200	-5.35758100	-0.43419100
H	-3.06973500	-3.92231200	-0.34651000
H	-1.46445100	-5.80948400	-0.23888100
C	-2.49981100	1.35629200	0.04527300
C	-3.30065900	1.11360100	-1.07447000
C	-2.91784900	2.29428600	0.99419500

C	-4.51058400	1.78174900	-1.22931400
H	-2.97211000	0.40046900	-1.82009000
C	-4.12640900	2.96019800	0.83626800
H	-2.28878400	2.52148800	1.84647200
C	-4.92802000	2.70315000	-0.27391000
H	-5.12683500	1.58151700	-2.09756100
H	-4.43821200	3.68897400	1.57467300
H	-5.86965900	3.22491800	-0.39624200
H	-1.14808300	0.69343300	2.33579600
Li	2.73978700	2.23365500	2.16229400

Zero-point correction= 0.337510 (Hartree/Particle)
 Thermal correction to Energy= 0.359426
 Thermal correction to Enthalpy= 0.360371
 Thermal correction to Gibbs Free Energy= 0.285833
 Sum of electronic and zero-point Energies= -1479.458568
 Sum of electronic and thermal Energies= -1479.436652
 Sum of electronic and thermal Enthalpies= -1479.435707
 Sum of electronic and thermal Free Energies= -1479.510245

11c

S	-0.97000000	-0.32787100	1.59669600
O	-0.84529200	-1.74705200	2.05790100
O	-1.68098600	0.51039800	2.57417100
C	0.66780400	0.29356600	1.45405200
H	1.13926300	0.61029400	2.37435700
C	1.21949000	0.54308400	0.24779000
C	-1.57923700	-0.20366300	0.01775700
C	-0.52863400	-0.60857300	-0.95908800
H	-0.92117100	-0.41696400	-1.95978600
O	0.68334400	0.23045900	-0.93959100
C	-2.41514900	0.96647900	-0.28806100
C	-3.59808100	1.22892400	0.43280700
C	-2.11010900	1.84248300	-1.34820900
C	-4.41582900	2.30501600	0.11894400
H	-3.87437700	0.56444000	1.24187000
C	-2.94970400	2.90308000	-1.68009600
H	-1.19354400	1.70895600	-1.91189000
C	-4.10572100	3.14970000	-0.94750100
H	-5.31679000	2.47430100	0.69862100
H	-2.68273100	3.55152900	-2.50756900
H	-4.75361200	3.98038100	-1.20040700
C	-0.09252000	-2.07078800	-0.92549300
C	1.24484300	-2.46115900	-0.90072300
C	-1.08353000	-3.05445000	-0.98460200
C	1.58562300	-3.81507700	-0.90789200
H	2.02944700	-1.71470000	-0.87699200
C	-0.74499200	-4.40168400	-1.00603800

H	-2.12337600	-2.74818900	-0.99649500
C	0.59505100	-4.78875900	-0.96042300
H	2.63024700	-4.10308400	-0.88067100
H	-1.52563500	-5.15199800	-1.05618500
H	0.86091100	-5.83921600	-0.97335800
C	2.52474600	1.23738500	0.10714800
C	3.50354600	1.14080200	1.09982000
C	2.78053800	1.99970000	-1.03608700
C	4.71183400	1.81318400	0.95961000
H	3.33173400	0.52257900	1.97288400
C	3.98773100	2.67633000	-1.16930500
H	2.02700100	2.06544900	-1.81075400
C	4.95566700	2.58597700	-0.17272100
H	5.46702800	1.72551000	1.73141300
H	4.17279400	3.27429700	-2.05360300
H	5.89821100	3.10922300	-0.28059000
Li	0.05929300	-3.33555500	2.16401500

Zero-point correction=	0.337169 (Hartree/Particle)
Thermal correction to Energy=	0.359249
Thermal correction to Enthalpy=	0.360193
Thermal correction to Gibbs Free Energy=	0.284599
Sum of electronic and zero-point Energies=	-1479.458787
Sum of electronic and thermal Energies=	-1479.436708
Sum of electronic and thermal Enthalpies=	-1479.435764
Sum of electronic and thermal Free Energies=	-1479.511358

11d

S	-0.95061400	0.30577500	1.58361800
O	-1.73938000	-0.69367400	2.37733100
O	-0.82372700	1.59140500	2.28726100
C	0.65749700	-0.38308500	1.41526900
C	1.21109700	-0.61126300	0.20586200
C	-1.50727200	0.38042700	-0.01902100
C	-0.39240100	0.78072500	-0.92170500
H	-0.76449400	0.74547500	-1.94734300
O	0.71771000	-0.18711200	-0.96574400
C	-2.48880300	-0.60609200	-0.46445800
C	-2.27648900	-1.40573300	-1.60766100
C	-3.72532200	-0.76870700	0.19990000
C	-3.24086800	-2.30143500	-2.05826600
H	-1.33476500	-1.33827600	-2.14065100
C	-4.67096900	-1.69042400	-0.23495200
H	-3.94897300	-0.13469600	1.05011500
C	-4.44183600	-2.46366500	-1.37249700
H	-3.03975300	-2.89346700	-2.94453700

H	-5.60874200	-1.78195600	0.30252400
H	-5.18682100	-3.16861400	-1.72073800
C	0.18177600	2.17787500	-0.69475900
C	1.54849500	2.43202000	-0.61229600
C	-0.70984200	3.25044700	-0.62272000
C	2.01597200	3.73527200	-0.44262200
H	2.26197000	1.61967600	-0.67438500
C	-0.24518000	4.54999200	-0.46949400
H	-1.77426600	3.05092300	-0.67069900
C	1.12347100	4.79759300	-0.37218900
H	3.08225300	3.91455400	-0.36788300
H	-0.95104400	5.37072800	-0.41626400
H	1.48769500	5.80980800	-0.24203000
C	2.48498100	-1.35705600	0.04448600
C	3.28275700	-1.12768200	-1.08019100
C	2.90032300	-2.29191700	0.99776000
C	4.48680900	-1.80618200	-1.23600800
H	2.95631300	-0.41692900	-1.82899900
C	4.10297800	-2.96817300	0.83892600
H	2.27364600	-2.50866400	1.85451100
C	4.90143200	-2.72463000	-0.27654100
H	5.10070300	-1.61641600	-2.10824900
H	4.41250000	-3.69441600	1.58078800
H	5.83836800	-3.25459000	-0.39971500
H	1.14495400	-0.67312700	2.33571300
Li	-2.38938800	-2.39906900	2.03608200

Zero-point correction= 0.337330 (Hartree/Particle)
 Thermal correction to Energy= 0.359310
 Thermal correction to Enthalpy= 0.360254
 Thermal correction to Gibbs Free Energy= 0.285552
 Sum of electronic and zero-point Energies= -1479.458761
 Sum of electronic and thermal Energies= -1479.436781
 Sum of electronic and thermal Enthalpies= -1479.435837
 Sum of electronic and thermal Free Energies= -1479.510539

11e

S	0.22609800	-2.18309500	-0.09581500
O	0.30068200	-3.01105200	1.16253000
O	0.69731500	-2.93676400	-1.27412000
C	-1.46041600	-1.77984500	-0.33306000
H	-2.08355600	-2.62876100	-0.57588500
C	-1.94747900	-0.55000400	-0.09840600
C	0.96748500	-0.66328700	0.27476800
C	0.19389000	0.47761000	-0.35587300
H	0.09472600	0.39889000	-1.45183000

O	-1.17868800	0.52359200	0.13332400
C	2.43376100	-0.73425500	0.00616500
C	3.24225900	-1.67453400	0.67344900
C	3.07332600	0.10047600	-0.92615900
C	4.60700500	-1.76618100	0.43204300
H	2.79387300	-2.35362400	1.39051000
C	4.44531500	0.02456100	-1.15071400
H	2.50053800	0.82181100	-1.49493400
C	5.22447400	-0.90753900	-0.47454400
H	5.19272100	-2.50623600	0.96560600
H	4.90185600	0.69295400	-1.87218600
H	6.29126500	-0.96854800	-0.65288800
C	0.73913400	1.85031600	-0.01779800
C	0.63073300	2.87449800	-0.95651400
C	1.29181400	2.12510200	1.23200800
C	1.08101500	4.15767000	-0.65850000
H	0.19913100	2.66351700	-1.92993300
C	1.74093000	3.40655300	1.53328100
H	1.37965600	1.32712200	1.96026200
C	1.63867200	4.42517500	0.58810400
H	0.99808300	4.94488800	-1.39846500
H	2.17498300	3.61109300	2.50500500
H	1.99350600	5.42188300	0.82251100
C	-3.39567600	-0.24118500	-0.07513400
C	-3.82970400	1.04632000	-0.40235200
C	-4.33380200	-1.21776300	0.27106800
C	-5.18733500	1.34506000	-0.40427900
H	-3.09988500	1.80325400	-0.66102500
C	-5.68951900	-0.91457200	0.26952600
H	-4.00382800	-2.20791600	0.56255500
C	-6.11913400	0.36606800	-0.07064000
H	-5.51771700	2.34285700	-0.66661400
H	-6.41046900	-1.67482800	0.54446800
H	-7.17673200	0.60136800	-0.06880700
Li	0.50643500	-1.48929200	2.41406100

Zero-point correction=	0.337177 (Hartree/Particle)
Thermal correction to Energy=	0.359435
Thermal correction to Enthalpy=	0.360379
Thermal correction to Gibbs Free Energy=	0.284406
Sum of electronic and zero-point Energies=	-1479.454916
Sum of electronic and thermal Energies=	-1479.432658
Sum of electronic and thermal Enthalpies=	-1479.431714
Sum of electronic and thermal Free Energies=	-1479.507687

S	-0.09011000	-1.97541500	-1.50631000
O	-0.00697400	-3.33958900	-0.89187700
O	-0.03296500	-1.99797800	-2.97998100
C	-1.64226800	-1.30397200	-1.04284600
H	-2.52163900	-1.92352600	-1.14807000
C	-1.69428900	-0.05511900	-0.52654500
C	1.06275100	-0.92976900	-0.82443800
C	0.58932000	0.45342000	-1.14895000
H	0.33695600	0.52693700	-2.21264400
O	-0.67274700	0.80487900	-0.44621600
C	1.47968200	-1.17833300	0.58706100
C	0.64291900	-1.69236200	1.59165100
C	2.78805200	-0.82751300	0.96185300
C	1.09729200	-1.86282000	2.89742700
H	-0.37956600	-1.96203800	1.35178700
C	3.23659700	-0.97174200	2.26999500
H	3.45364100	-0.42981500	0.20291900
C	2.39426200	-1.49858100	3.24684800
H	0.42663600	-2.26666500	3.64796800
H	4.25071600	-0.68415500	2.52437800
H	2.74388500	-1.62268900	4.26510500
C	1.57412500	1.53977600	-0.79372900
C	1.50700900	2.23005800	0.41395400
C	2.61881500	1.80915900	-1.67808700
C	2.48057500	3.17294600	0.73715000
H	0.69778600	2.02256900	1.10319600
C	3.59107300	2.74903800	-1.35617000
H	2.67392100	1.26711100	-2.61685200
C	3.52576800	3.43303600	-0.14331000
H	2.42206600	3.70225400	1.68121300
H	4.39820200	2.94976200	-2.05101100
H	4.28271200	4.16603200	0.10977100
C	-2.95278800	0.51610700	0.01650600
C	-3.16539500	1.89616200	-0.03856000
C	-3.92827600	-0.30634500	0.58652700
C	-4.34731700	2.44167700	0.45002100
H	-2.40448100	2.53287900	-0.47199000
C	-5.10727000	0.24234100	1.07642000
H	-3.75595300	-1.37312200	0.66775200
C	-5.32108600	1.61687700	1.00623900
H	-4.50796800	3.51173200	0.39572100
H	-5.85472700	-0.40213900	1.52317400
H	-6.24025600	2.04336900	1.38990400
Li	1.51467400	-4.34486700	-0.48362300

Zero-point correction=	0.336360 (Hartree/Particle)
Thermal correction to Energy=	0.358892
Thermal correction to Enthalpy=	0.359836

Thermal correction to Gibbs Free Energy=	0.282612
Sum of electronic and zero-point Energies=	-1479.457720
Sum of electronic and thermal Energies=	-1479.435188
Sum of electronic and thermal Enthalpies=	-1479.434244
Sum of electronic and thermal Free Energies=	-1479.511468

11g

S	0.14304300	-1.83624700	-1.59410300
O	0.35313200	-3.20979900	-1.03776900
O	0.20239800	-1.80245000	-3.06472900
C	-1.47944300	-1.35457100	-1.10705700
H	-2.27679700	-2.05939700	-1.29940800
C	-1.69668700	-0.18741300	-0.46144500
C	1.13608400	-0.69286100	-0.82202100
C	0.48396600	0.62881500	-1.02105700
H	0.17798000	0.72427900	-2.07168100
O	-0.79004200	0.77906700	-0.27678400
C	1.73808300	-1.06311200	0.46202600
C	1.52055300	-0.31721400	1.63834100
C	2.61501600	-2.16461900	0.56090000
C	2.14011300	-0.65684800	2.83705700
H	0.85213300	0.53508400	1.61285400
C	3.20558200	-2.52032900	1.76873900
H	2.85061400	-2.72550100	-0.33633800
C	2.97700300	-1.76672700	2.91913100
H	1.95249300	-0.05464100	3.71937800
H	3.87445500	-3.37359800	1.80338700
H	3.45194900	-2.03222800	3.85590100
C	1.33355800	1.83583500	-0.67277000
C	0.76953700	2.99718500	-0.14426900
C	2.70363100	1.80802700	-0.93835100
C	1.56518500	4.10969200	0.11994800
H	-0.29076200	3.02996300	0.06994700
C	3.49554000	2.92227700	-0.68159400
H	3.14282300	0.90261900	-1.34040500
C	2.92973500	4.07763800	-0.14842600
H	1.11428200	5.00309400	0.53623900
H	4.55799600	2.88496200	-0.89245900
H	3.54754900	4.94383800	0.05702700
C	-3.02189100	0.16282800	0.10846600
C	-3.41211300	1.50302600	0.17443300
C	-3.88627300	-0.82728500	0.58282400
C	-4.65709000	1.84486400	0.69033100
H	-2.74059000	2.27013000	-0.19014200
C	-5.12910200	-0.48242000	1.10013700
H	-3.57771600	-1.86591600	0.56771700

C	-5.51849300	0.85379700	1.15259500
H	-4.95496400	2.88572400	0.73030700
H	-5.78969000	-1.25616500	1.47239100
H	-6.48698100	1.12134300	1.55801200
Li	0.43588500	-3.98389500	0.65985200

Zero-point correction= 0.337058 (Hartree/Particle)
 Thermal correction to Energy= 0.359219
 Thermal correction to Enthalpy= 0.360164
 Thermal correction to Gibbs Free Energy= 0.284623
 Sum of electronic and zero-point Energies= -1479.460880
 Sum of electronic and thermal Energies= -1479.438719
 Sum of electronic and thermal Enthalpies= -1479.437775
 Sum of electronic and thermal Free Energies= -1479.513315

11h

S	-0.12352600	-2.09052600	-1.24266600
O	-0.08169800	-3.42390700	-0.56758200
O	-0.03004600	-2.33420400	-2.72105300
C	-1.66251000	-1.32860200	-0.92281600
H	-2.55486400	-1.93229600	-1.00787800
C	-1.69341000	-0.04578400	-0.48609300
C	1.04204500	-1.00901800	-0.67501000
C	0.59399000	0.34492800	-1.12839700
H	0.32916000	0.32168300	-2.19221300
O	-0.65329200	0.78846600	-0.45425700
C	1.49152200	-1.14863500	0.73987300
C	0.66706800	-1.56706100	1.79543400
C	2.81093200	-0.78717000	1.05623200
C	1.14452000	-1.63780800	3.10171300
H	-0.36205000	-1.84470300	1.59494600
C	3.28292900	-0.83119800	2.36322100
H	3.46645900	-0.46385600	0.25458500
C	2.45271200	-1.26447400	3.39480000
H	0.48521400	-1.97287700	3.89472000
H	4.30580600	-0.54011800	2.57461100
H	2.82143900	-1.31150200	4.41277100
C	1.60827800	1.43564400	-0.89307400
C	1.58656500	2.22921600	0.25102500
C	2.63481700	1.60076800	-1.82270500
C	2.58922100	3.17243200	0.46652700
H	0.79163800	2.10097700	0.97555000
C	3.63612300	2.54044600	-1.60750200

H	2.65349500	0.97800900	-2.71142200
C	3.61698400	3.32852600	-0.45804400
H	2.56759400	3.78293600	1.36179900
H	4.42962900	2.65983000	-2.33586500
H	4.39673000	4.06146700	-0.28773400
C	-2.94398900	0.58653600	0.00117700
C	-3.11867200	1.96630900	-0.13517600
C	-3.94648100	-0.17801300	0.60408100
C	-4.29070000	2.56853200	0.30790200
H	-2.33636100	2.55753900	-0.59422400
C	-5.11543100	0.42781600	1.04798500
H	-3.80251400	-1.24223600	0.74874700
C	-5.29130400	1.80136600	0.89805400
H	-4.42257300	3.63761500	0.19256100
H	-5.88427200	-0.17037600	1.52184500
H	-6.20250400	2.27258000	1.24679000
Li	0.28114300	-4.30587500	-2.40634600

Zero-point correction= 0.336562 (Hartree/Particle)
 Thermal correction to Energy= 0.358922
 Thermal correction to Enthalpy= 0.359866
 Thermal correction to Gibbs Free Energy= 0.283174
 Sum of electronic and zero-point Energies= -1479.457554
 Sum of electronic and thermal Energies= -1479.435194
 Sum of electronic and thermal Enthalpies= -1479.434250
 Sum of electronic and thermal Free Energies= -1479.510942

Transition States for Ring Opening:

11a[‡]

S	-0.98072700	0.10765800	1.52246600
O	-1.79300600	-0.97987200	2.16231000
O	-1.02609900	1.26323000	2.48186800
C	0.63723400	-0.40555200	1.27999900
C	1.19591100	-0.69885200	0.04820500
C	-1.58044600	0.40559500	-0.07356000
C	-0.63043100	0.90906800	-0.96052400
H	-0.91873700	0.81020200	-2.00432600
O	0.75406900	-0.36850100	-1.10922800
C	-2.68456400	-0.46285900	-0.54093700
C	-2.52252500	-1.29213800	-1.65888700
C	-3.93171000	-0.45204200	0.09825900
C	-3.57774900	-2.06647400	-2.13320600
H	-1.55560900	-1.34107800	-2.14780100
C	-4.97866500	-1.24078500	-0.36272900

H	-4.07889900	0.19240000	0.95778700
C	-4.80948600	-2.04822400	-1.48609300
H	-3.42989000	-2.69749000	-3.00218000
H	-5.93510400	-1.21421200	0.14691700
H	-5.62902800	-2.65546500	-1.85158000
C	0.22539000	2.11475200	-0.71618800
C	-0.17515800	3.10601400	0.18045700
C	1.37530400	2.32646900	-1.48771600
C	0.58353100	4.26434600	0.33811300
H	-1.08249400	2.97118700	0.75316200
C	2.13096300	3.47965400	-1.32886800
H	1.67415700	1.57389700	-2.20647600
C	1.74082300	4.45149200	-0.40758100
H	0.26232600	5.02186500	1.04337700
H	3.02226300	3.62531100	-1.92781800
H	2.33007200	5.35257500	-0.28430700
C	2.50297600	-1.43102100	0.04105800
C	3.42318100	-1.14719300	-0.97092000
C	2.81696500	-2.39332900	1.00329100
C	4.65038300	-1.79892900	-1.00650000
H	3.16685300	-0.40975500	-1.72162400
C	4.04068000	-3.05310500	0.95988400
H	2.09476300	-2.64462300	1.77123300
C	4.96137500	-2.75336600	-0.04088700
H	5.36349200	-1.56468500	-1.78794400
H	4.27224800	-3.80698400	1.70284700
H	5.91504500	-3.26692900	-0.07212900
H	1.15427700	-0.63577400	2.20063800
Li	-2.25924100	0.25568300	3.71438600

Zero-point correction= 0.334559 (Hartree/Particle)
 Thermal correction to Energy= 0.356912
 Thermal correction to Enthalpy= 0.357856
 Thermal correction to Gibbs Free Energy= 0.281198
 Sum of electronic and zero-point Energies= -1479.449625
 Sum of electronic and thermal Energies= -1479.427272
 Sum of electronic and thermal Enthalpies= -1479.426328
 Sum of electronic and thermal Free Energies= -1479.502986

Imaginary Frequency: -359.61 cm⁻¹

11b⁺

S	0.73294300	0.79480400	1.57324900
O	0.30053300	2.01548600	2.32357600
O	1.87149500	0.11173000	2.19939700
C	-0.66586800	-0.22323600	1.46637100
C	-0.94040000	-0.95329600	0.33595800

C	1.01511200	1.18469300	-0.09288200
C	1.24864800	0.03095600	-0.86201100
H	1.04576400	0.18947600	-1.91982200
O	-0.15275300	-1.14340400	-0.67276700
C	0.13472500	2.25291300	-0.62914800
C	-0.92981500	1.96565900	-1.49618600
C	0.36674600	3.59616400	-0.29540600
C	-1.72513400	2.98394400	-2.01605700
H	-1.13914400	0.93339900	-1.75754400
C	-0.44278900	4.61113300	-0.79520000
H	1.20178000	3.83516300	0.35403300
C	-1.49133800	4.30965800	-1.66307200
H	-2.53879000	2.73741800	-2.68879000
H	-0.24076000	5.64175700	-0.52573500
H	-2.11405900	5.10075900	-2.06369500
C	2.40565400	-0.90455000	-0.65559100
C	3.60438100	-0.42145000	-0.12799300
C	2.35483500	-2.22395800	-1.11552500
C	4.72154300	-1.24594000	-0.03676700
H	3.65158300	0.60329600	0.21606300
C	3.47039900	-3.04883800	-1.02053200
H	1.43284000	-2.60366900	-1.53583900
C	4.65813800	-2.56369600	-0.47869100
H	5.64231800	-0.85619600	0.38149800
H	3.41253900	-4.07181500	-1.37391900
H	5.52791400	-3.20626300	-0.40708100
C	-2.27527400	-1.62510100	0.21669000
C	-2.36543200	-2.81374200	-0.51194200
C	-3.42910800	-1.09392600	0.79844500
C	-3.58425700	-3.47061900	-0.64034200
H	-1.47022500	-3.21712400	-0.96951700
C	-4.64947700	-1.74746600	0.66323300
H	-3.38023700	-0.15527000	1.33774100
C	-4.72930600	-2.93952000	-0.05215700
H	-3.64090100	-4.39725400	-1.19922500
H	-5.54018200	-1.32092000	1.10919200
H	-5.68024600	-3.44864700	-0.15538700
H	-1.37217000	-0.12554000	2.27738500
Li	-1.06373300	3.27179100	2.33328200

Zero-point correction=	0.335017 (Hartree/Particle)
Thermal correction to Energy=	0.357131
Thermal correction to Enthalpy=	0.358076
Thermal correction to Gibbs Free Energy=	0.282495
Sum of electronic and zero-point Energies=	-1479.449317
Sum of electronic and thermal Energies=	-1479.427203
Sum of electronic and thermal Enthalpies=	-1479.426258
Sum of electronic and thermal Free Energies=	-1479.501839

Imaginary Frequency:

-317.88 cm⁻¹

11c⁺

S	-0.73758600	0.78874900	1.60050000
O	-1.92811300	-0.02100100	1.99335900
O	-0.45171000	1.91924400	2.49564100
C	0.67232800	-0.22258400	1.54512400
H	1.45464700	0.03952200	2.24225500
C	0.90441600	-0.98423300	0.42695200
C	-0.89070800	1.24571100	-0.05945600
C	-1.14585600	0.11605000	-0.87092500
H	-0.83088600	0.27554800	-1.90091900
O	0.05483100	-1.18117400	-0.53544300
C	0.13593500	2.22916000	-0.49067600
C	0.08661900	3.55453300	-0.03444400
C	1.17122300	1.87709700	-1.36990300
C	1.02969300	4.48988700	-0.44341600
H	-0.70573200	3.84314100	0.64570300
C	2.10402700	2.81878700	-1.79567600
H	1.25802400	0.85182900	-1.71485000
C	2.04048800	4.12946800	-1.33270900
H	0.96809600	5.50826800	-0.07667200
H	2.89151400	2.52115200	-2.47890100
H	2.76985000	4.86155800	-1.65863700
C	-2.42491100	-0.67335500	-0.82292100
C	-2.47778800	-1.99284000	-1.27933200
C	-3.61304100	-0.04285300	-0.44903400
C	-3.68966000	-2.67519000	-1.33032500
H	-1.56424500	-2.48660900	-1.58326000
C	-4.82531300	-0.72328100	-0.50412800
H	-3.57453100	0.98412200	-0.10869000
C	-4.86838600	-2.04428800	-0.94146400
H	-3.71283100	-3.70062600	-1.68089600
H	-5.73766600	-0.21894800	-0.20687300
H	-5.81241100	-2.57474400	-0.98693100
C	2.24227400	-1.62401000	0.23549100
C	3.04383800	-1.98673100	1.32086100
C	2.69992800	-1.86975400	-1.06158600
C	4.29160400	-2.56364100	1.11109200
H	2.68456300	-1.83768900	2.33254000
C	3.95185200	-2.43745100	-1.26987800
H	2.06682100	-1.60841000	-1.90080400
C	4.75195400	-2.78536400	-0.18438200
H	4.90174100	-2.84757200	1.96036600

H	4.30229100	-2.61194500	-2.28036100
H	5.72459100	-3.23447700	-0.34657600
Li	-2.60854700	-1.04378900	3.37049300

Zero-point correction=	0.334759 (Hartree/Particle)
Thermal correction to Energy=	0.357050
Thermal correction to Enthalpy=	0.357994
Thermal correction to Gibbs Free Energy=	0.281872
Sum of electronic and zero-point Energies=	-1479.450893
Sum of electronic and thermal Energies=	-1479.428602
Sum of electronic and thermal Enthalpies=	-1479.427658
Sum of electronic and thermal Free Energies=	-1479.503781

Imaginary Frequency	-320.29 cm ⁻¹
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11d[‡]

S	-0.97566600	0.19936500	1.59022200
O	-1.84068600	-0.89013800	2.15450000
O	-0.88838200	1.33632700	2.52133000
C	0.59749500	-0.45963100	1.30235200
C	1.13409400	-0.72787100	0.06221100
C	-1.57288100	0.56042100	-0.00864400
C	-0.59686000	1.02016300	-0.89116900
H	-0.89410500	0.96207300	-1.93561900
O	0.69489100	-0.34381700	-1.08650700
C	-2.69469200	-0.27094000	-0.49363000
C	-2.55641500	-1.09173900	-1.62345700
C	-3.94077900	-0.24848500	0.15370500
C	-3.62868100	-1.84152400	-2.10020400
H	-1.59369800	-1.15078600	-2.11927400
C	-5.00413100	-1.01521400	-0.31021900
H	-4.07141500	0.38983500	1.02038700
C	-4.85601500	-1.81214100	-1.44464700
H	-3.49772100	-2.46258700	-2.97912200
H	-5.95741500	-0.97560200	0.20458600
H	-5.68850300	-2.39948800	-1.81329500
C	0.32853100	2.16991800	-0.62745500
C	1.50029500	2.31929600	-1.38037700
C	-0.02870400	3.17992500	0.26706200
C	2.31673500	3.42845900	-1.20670600
H	1.76666700	1.55340000	-2.09755600
C	0.79051800	4.29379700	0.43940100
H	-0.94900200	3.09222500	0.82802600

C	1.96745000	4.41850900	-0.28879300
H	3.22398600	3.52505500	-1.79158100
H	0.50177500	5.06552200	1.14328500
H	2.60409300	5.28501600	-0.15359300
C	2.41362700	-1.50911600	0.01701600
C	3.32816200	-1.23915500	-1.00385800
C	2.71022500	-2.50224500	0.95358300
C	4.53091900	-1.93306300	-1.07304900
H	3.08676200	-0.47832400	-1.73570800
C	3.90935800	-3.20313200	0.87802000
H	1.99362900	-2.74277200	1.73023000
C	4.82443800	-2.91673100	-0.13183000
H	5.23894700	-1.70810400	-1.86191100
H	4.12603000	-3.97841500	1.60339000
H	5.75881200	-3.46255800	-0.18872700
H	1.11552300	-0.73040600	2.21158000
Li	-2.57214800	-2.50330400	1.61363000

Zero-point correction= 0.334986 (Hartree/Particle)
 Thermal correction to Energy= 0.357162
 Thermal correction to Enthalpy= 0.358106
 Thermal correction to Gibbs Free Energy= 0.282244
 Sum of electronic and zero-point Energies= -1479.449379
 Sum of electronic and thermal Energies= -1479.427203
 Sum of electronic and thermal Enthalpies= -1479.426259
 Sum of electronic and thermal Free Energies= -1479.502121

Imaginary Frequency -353.59 cm⁻¹

11e⁺

S	0.17398200	-2.19128900	-0.18443500
O	0.15857300	-2.45164800	1.30615800
O	0.59312200	-3.37182500	-0.95445500
C	-1.49967500	-1.78035000	-0.56158900
H	-2.05823400	-2.50163300	-1.13849900
C	-1.96894400	-0.66052500	0.02603400
C	1.05931900	-0.74492100	-0.46270300
C	0.19122600	0.40494800	-0.54169500
H	-0.49879200	0.44372300	-1.38638100
O	-1.09905100	0.19500600	0.59629900
C	2.51028200	-0.77190100	-0.26074100
C	3.16201400	-1.74683700	0.51989300
C	3.33039900	0.17230500	-0.91348200
C	4.54781800	-1.76400900	0.64736600
H	2.58064300	-2.49692400	1.04192200
C	4.70882000	0.17086100	-0.75562200

H	2.87269500	0.91089000	-1.56135500
C	5.33460700	-0.80027900	0.02554200
H	5.01188200	-2.53417500	1.25365600
H	5.30184900	0.92006500	-1.26855400
H	6.41217300	-0.81044600	0.13590900
C	0.72334700	1.75873700	-0.21817800
C	0.40254600	2.82981200	-1.05145500
C	1.49401400	1.98801200	0.92523700
C	0.86845400	4.11079400	-0.76646900
H	-0.20822100	2.65772100	-1.93139200
C	1.94358500	3.26765700	1.22032700
H	1.75951200	1.15973800	1.57316500
C	1.63795900	4.33098700	0.37062000
H	0.62451200	4.93385200	-1.42734000
H	2.54005100	3.43813300	2.10865600
H	1.99692900	5.32756000	0.59901800
C	-3.39121500	-0.26063400	0.03986600
C	-3.71863900	1.09285200	0.15779200
C	-4.41066900	-1.21141800	-0.07295200
C	-5.05058600	1.49160000	0.14214600
H	-2.92270300	1.82155500	0.25255200
C	-5.73971800	-0.80934700	-0.08574800
H	-4.16310600	-2.26502100	-0.13122800
C	-6.06190900	0.54272000	0.01923600
H	-5.29952200	2.54265200	0.22586700
H	-6.52568500	-1.55024400	-0.16810200
H	-7.09974400	0.85382700	0.01141900
Li	-0.25577500	-0.80976700	2.25236100

Zero-point correction=	0.335715 (Hartree/Particle)
Thermal correction to Energy=	0.357596
Thermal correction to Enthalpy=	0.358540
Thermal correction to Gibbs Free Energy=	0.284142
Sum of electronic and zero-point Energies=	-1479.438068
Sum of electronic and thermal Energies=	-1479.416187
Sum of electronic and thermal Enthalpies=	-1479.415243
Sum of electronic and thermal Free Energies=	-1479.489642

Imaginary Frequency	-469.03 cm ⁻¹
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11f*

S	-0.11391600	-1.88634400	-1.59081200
O	0.00732400	-3.27644700	-1.04740100
O	-0.02414000	-1.82578600	-3.06139600
C	-1.62560000	-1.25260000	-1.03629700
H	-2.44803300	-1.95069500	-0.99199900

C	-1.72771700	0.03972500	-0.58612700
C	1.05830100	-0.85497300	-0.85748700
C	0.78390900	0.46925500	-1.26104700
H	0.51066900	0.58647800	-2.30754600
O	-0.82406400	0.97002500	-0.65446000
C	1.57458600	-1.19757700	0.49259500
C	0.77343100	-1.71959200	1.51902200
C	2.92741400	-0.95948600	0.77667300
C	1.30646800	-1.99406300	2.77568600
H	-0.27929300	-1.90285700	1.33316800
C	3.45607800	-1.21130500	2.03787300
H	3.56085100	-0.55987400	-0.00815500
C	2.64784600	-1.73529600	3.04432600
H	0.66577000	-2.39617700	3.55251100
H	4.50304600	-1.00770100	2.23216100
H	3.05871000	-1.93965700	4.02604200
C	1.61683200	1.59779500	-0.74776500
C	1.57039900	1.99520000	0.58936800
C	2.48983900	2.24207600	-1.62299200
C	2.39771000	3.01453000	1.04495900
H	0.88089600	1.50240700	1.26450200
C	3.32646900	3.25703300	-1.16477200
H	2.52048000	1.94219700	-2.66528600
C	3.28235900	3.64442400	0.17058600
H	2.35341800	3.31938700	2.08402000
H	4.00511200	3.74754600	-1.85257400
H	3.92788100	4.43788100	0.52840500
C	-3.00929700	0.47648800	0.05344000
C	-3.40065400	1.81252000	-0.06237100
C	-3.81495200	-0.41107300	0.77108300
C	-4.58991200	2.24910800	0.51061500
H	-2.76665200	2.49907900	-0.60954100
C	-5.00068100	0.02847000	1.34999300
H	-3.50460200	-1.44162600	0.89831800
C	-5.39335500	1.35788200	1.21720100
H	-4.88974900	3.28515400	0.40629600
H	-5.61358300	-0.66534800	1.91306400
H	-6.31810400	1.69859200	1.66771100
Li	1.49535300	-4.33561900	-0.66646900

Zero-point correction=	0.334669 (Hartree/Particle)
Thermal correction to Energy=	0.357107
Thermal correction to Enthalpy=	0.358052
Thermal correction to Gibbs Free Energy=	0.280933
Sum of electronic and zero-point Energies=	-1479.453266
Sum of electronic and thermal Energies=	-1479.430828
Sum of electronic and thermal Enthalpies=	-1479.429884
Sum of electronic and thermal Free Energies=	-1479.507002

Imaginary Frequency

-344.27 cm⁻¹**11g⁺**

S	0.07014200	-1.75484500	-1.73712400
O	0.23403400	-3.17162700	-1.28264300
O	0.17183800	-1.60198400	-3.19691500
C	-1.46915700	-1.21267900	-1.14710100
H	-2.26521900	-1.94112100	-1.19359000
C	-1.64511700	0.02399400	-0.57531900
C	1.18409500	-0.72504900	-0.90160900
C	0.84942400	0.60508500	-1.20482400
H	0.51419500	0.76779900	-2.22749100
O	-0.79403600	1.00011100	-0.53055300
C	1.59395900	-1.17550300	0.44641600
C	1.15801900	-0.51297500	1.60459800
C	2.44783000	-2.27893100	0.60066600
C	1.56974900	-0.93266900	2.86582000
H	0.49329000	0.33813900	1.50462100
C	2.84117500	-2.71168100	1.86415200
H	2.81625100	-2.78318200	-0.28599900
C	2.40708500	-2.03698400	3.00340300
H	1.22591900	-0.40099800	3.74585400
H	3.50509500	-3.56376800	1.95744600
H	2.72348700	-2.36482700	3.98651200
C	1.64840500	1.75277400	-0.66820700
C	1.09322100	3.03329800	-0.60002800
C	2.98574300	1.57520300	-0.30686000
C	1.85380100	4.10883700	-0.15465900
H	0.05889300	3.17679600	-0.88545400
C	3.74772900	2.65324600	0.13369700
H	3.43211000	0.59079500	-0.37960000
C	3.18303900	3.92209900	0.21701800
H	1.40844900	5.09535800	-0.10072400
H	4.78428900	2.49962200	0.40992900
H	3.77558900	4.76103000	0.56252600
C	-2.96163600	0.33180100	0.07230800
C	-3.40878600	1.65530100	0.08914000
C	-3.74508100	-0.65941700	0.66849000
C	-4.62879400	1.97897200	0.67239300
H	-2.79263900	2.42259400	-0.36332800
C	-4.96177700	-0.33365100	1.25822900
H	-3.39462100	-1.68440500	0.69387100
C	-5.40885400	0.98510900	1.25769600
H	-4.97070000	3.00720300	0.67106800
H	-5.55675000	-1.10874800	1.72656500
H	-6.35740000	1.23739900	1.71677900

Li	0.19279500	-4.02041900	0.38779300
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Zero-point correction=	0.335051 (Hartree/Particle)
Thermal correction to Energy=	0.357264
Thermal correction to Enthalpy=	0.358208
Thermal correction to Gibbs Free Energy=	0.282225
Sum of electronic and zero-point Energies=	-1479.455450
Sum of electronic and thermal Energies=	-1479.433237
Sum of electronic and thermal Enthalpies=	-1479.432293
Sum of electronic and thermal Free Energies=	-1479.508276

Imaginary Frequency	-335.74 cm ⁻¹
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11h⁺

S	0.15326100	-1.98560300	1.35379200
O	0.05401900	-3.35106600	0.75448400
O	0.04357000	-2.14115700	2.84326100
C	1.65094600	-1.26045700	0.91865800
H	2.50654800	-1.91925400	0.91267500
C	1.73075400	0.05004900	0.50167500
C	-1.03956900	-0.91651300	0.73651800
C	-0.76495900	0.38007000	1.21627800
H	-0.43601000	0.43301000	2.25340800
O	0.80311200	0.94834000	0.56480600
C	-1.61754300	-1.19185800	-0.60399600
C	-0.84656100	-1.60713200	-1.69752200
C	-2.98896400	-0.98753100	-0.80395800
C	-1.42830300	-1.81416200	-2.94477700
H	0.21953100	-1.76399900	-1.57091800
C	-3.56821200	-1.17201800	-2.05459800
H	-3.59683700	-0.66950600	0.03626300
C	-2.79005200	-1.59117300	-3.13105900
H	-0.81279400	-2.13814800	-3.77630900
H	-4.63023500	-0.99893400	-2.18617700
H	-3.24061300	-1.74457900	-4.10460300
C	-1.63774200	1.52563000	0.82304500
C	-1.68289800	1.99212500	-0.49183600
C	-2.45031000	2.11734100	1.78855200
C	-2.54095600	3.02955500	-0.83539500
H	-1.04067000	1.53901900	-1.23776200
C	-3.31784600	3.15049700	1.44219600
H	-2.40966500	1.76308400	2.81324000
C	-3.36500200	3.60756300	0.12928900
H	-2.56843600	3.38875100	-1.85747400
H	-3.94945500	3.60041200	2.19900300
H	-4.03506700	4.41495500	-0.14166400
C	3.02212700	0.53461700	-0.07871700

C	3.37262000	1.87730300	0.08158700
C	3.87267000	-0.31551600	-0.78961200
C	4.56732800	2.35774800	-0.44233600
H	2.70324500	2.53400200	0.62325500
C	5.06352900	0.16872000	-1.32002300
H	3.59291300	-1.34987800	-0.95156500
C	5.41552800	1.50433500	-1.14347300
H	4.83623100	3.39833900	-0.30503500
H	5.71195000	-0.49480700	-1.87963300
H	6.34422100	1.87984700	-1.55662600
Li	-0.26404900	-4.12892100	2.65528700

Zero-point correction= 0.334604 (Hartree/Particle)
 Thermal correction to Energy= 0.356994
 Thermal correction to Enthalpy= 0.357938
 Thermal correction to Gibbs Free Energy= 0.280991
 Sum of electronic and zero-point Energies= -1479.453380
 Sum of electronic and thermal Energies= -1479.430990
 Sum of electronic and thermal Enthalpies= -1479.430046
 Sum of electronic and thermal Free Energies= -1479.506993

Imaginary Frequency -351.33 cm⁻¹

Ring Opened Products - E and Z Keto Sulfone:

12Za

S	-1.10258000	0.07007400	1.44408600
O	-1.98759900	-1.03602400	1.91021500
O	-1.35845800	1.27317100	2.29923200
C	0.54211600	-0.28618000	1.46156600
C	1.03076300	-1.22318700	0.52488000
C	-1.68018000	0.43824500	-0.23577300
C	-0.90250000	1.01449600	-1.15582000
H	-1.34404500	1.10043200	-2.14811600
O	0.30337800	-1.93932400	-0.18501300
C	-3.06160400	-0.01549800	-0.53270500
C	-3.28421500	-0.97662700	-1.51897700
C	-4.14976900	0.52642400	0.15694200
C	-4.58102400	-1.38461700	-1.81953200
H	-2.43662500	-1.40808600	-2.03941500
C	-5.44307900	0.11588100	-0.14218800
H	-3.97777700	1.28009000	0.91853700
C	-5.66125200	-0.84089300	-1.13191900
H	-4.74497300	-2.13158700	-2.58712200
H	-6.28220900	0.54638700	0.39135400

H	-6.67005600	-1.16043400	-1.36460900
C	0.46822900	1.55176700	-1.02949400
C	0.79652900	2.49871100	-0.05491500
C	1.44769600	1.13317700	-1.93320800
C	2.09178800	2.99473600	0.03045500
H	0.03464300	2.83316200	0.64089100
C	2.74793600	1.61771300	-1.83555600
H	1.19409500	0.40503800	-2.69649100
C	3.07270100	2.54908500	-0.85396300
H	2.33767100	3.72761500	0.78996900
H	3.50653700	1.26552800	-2.52470000
H	4.08435800	2.93054100	-0.78042800
C	2.52905900	-1.30663800	0.35412000
C	3.02125200	-1.89735600	-0.81099500
C	3.43111700	-0.79062800	1.28674700
C	4.38854800	-1.95032000	-1.05443500
H	2.31254300	-2.29890500	-1.52521400
C	4.80105000	-0.84890000	1.04849000
H	3.07171700	-0.35172100	2.21006100
C	5.28268400	-1.42147700	-0.12583200
H	4.75856900	-2.40037700	-1.96841600
H	5.49249200	-0.44851400	1.78066100
H	6.34945000	-1.46116100	-0.31310800
H	1.12975000	0.50215100	1.90222000
Li	-2.72016600	0.19286700	3.41525500

Zero-point correction= 0.334112 (Hartree/Particle)
 Thermal correction to Energy= 0.357679
 Thermal correction to Enthalpy= 0.358623
 Thermal correction to Gibbs Free Energy= 0.278975
 Sum of electronic and zero-point Energies= -1479.484502
 Sum of electronic and thermal Energies= -1479.460935
 Sum of electronic and thermal Enthalpies= -1479.459991
 Sum of electronic and thermal Free Energies= -1479.539639

12Zb

S	0.51639300	0.19221000	1.47857000
O	0.49241100	1.34880100	2.43215000
O	1.42710800	-0.87787400	1.88691300
C	-1.10485400	-0.25748300	1.25084400
C	-1.44963000	-1.14521500	0.22249700
C	1.14563700	0.92676800	-0.04849500
C	2.22241800	0.50792300	-0.72206700
H	2.51897200	1.17664200	-1.53087900
O	-0.62765900	-1.72008100	-0.52041900
C	0.43763800	2.18109700	-0.42753300

C	-0.83487500	2.14198800	-1.00520300
C	1.05799000	3.41643200	-0.22236400
C	-1.47451500	3.32320100	-1.36907900
H	-1.31054000	1.18490800	-1.18407400
C	0.41582400	4.59663000	-0.58622100
H	2.04548100	3.44401700	0.22510700
C	-0.85361500	4.55154600	-1.15631200
H	-2.45585400	3.28265600	-1.82698900
H	0.90751900	5.54893600	-0.42605600
H	-1.35385600	5.46946800	-1.44158400
C	3.09898000	-0.67538100	-0.59045700
C	4.48003300	-0.47884600	-0.69488100
C	2.59984400	-1.97510000	-0.46708300
C	5.35550200	-1.55727800	-0.62502300
H	4.86903200	0.52606500	-0.82253100
C	3.47732000	-3.05245400	-0.42090100
H	1.52800800	-2.12310600	-0.41355700
C	4.85413600	-2.84862900	-0.48818900
H	6.42415900	-1.39018000	-0.68952200
H	3.08404500	-4.05846700	-0.33075400
H	5.53219100	-3.69300900	-0.44538600
C	-2.92156000	-1.39963900	-0.00507900
C	-3.29844900	-2.61385200	-0.58261000
C	-3.90780200	-0.46083700	0.30613600
C	-4.63808000	-2.89643400	-0.82350700
H	-2.52541300	-3.32916000	-0.83663700
C	-5.24857600	-0.73691300	0.05315100
H	-3.63059400	0.50003900	0.72441200
C	-5.61715500	-1.95733300	-0.50607900
H	-4.91995000	-3.84668100	-1.26184200
H	-6.00474500	0.00308700	0.28786900
H	-6.66136000	-2.17321800	-0.69958000
H	-1.79753500	0.26343600	1.89138800
Li	-0.54133400	2.86376400	2.72836000

Zero-point correction=	0.334611 (Hartree/Particle)
Thermal correction to Energy=	0.358126
Thermal correction to Enthalpy=	0.359070
Thermal correction to Gibbs Free Energy=	0.279179
Sum of electronic and zero-point Energies=	-1479.480726
Sum of electronic and thermal Energies=	-1479.457211
Sum of electronic and thermal Enthalpies=	-1479.456267
Sum of electronic and thermal Free Energies=	-1479.536158

12Zc

S	-0.77216900	-0.59844600	1.21239400
O	-1.52781500	-1.71258100	0.58039600

O	-1.15514900	-0.26063800	2.58996200
C	0.90588500	-0.90117700	1.14174300
H	1.45996300	-0.53858700	1.99256700
C	1.45992200	-1.22391800	-0.09088900
C	-1.06317400	0.86298500	0.16854400
C	-2.20003400	1.07886100	-0.50188700
H	-2.19045900	1.95666500	-1.14742900
O	0.78147300	-1.45177500	-1.13875300
C	0.10088800	1.78068600	0.07853100
C	0.61282100	2.39165900	1.22715800
C	0.70697400	2.02075000	-1.15525100
C	1.71213900	3.23666100	1.13752600
H	0.14716200	2.19921500	2.18801700
C	1.80762500	2.86892600	-1.24216600
H	0.32361200	1.52540100	-2.04006900
C	2.31325500	3.47589900	-0.09699700
H	2.10042900	3.70990600	2.03154900
H	2.27449100	3.04659800	-2.20380700
H	3.17311200	4.13171000	-0.16391200
C	-3.47719200	0.34202200	-0.49218200
C	-4.17278600	0.19380900	-1.69699200
C	-4.05158600	-0.14179900	0.68760100
C	-5.39429200	-0.46960700	-1.73149600
H	-3.74797000	0.59556600	-2.61087600
C	-5.27982400	-0.79012800	0.65427400
H	-3.53841000	-0.00070600	1.63184300
C	-5.94987700	-0.96445900	-0.55479700
H	-5.91649700	-0.58940800	-2.67322600
H	-5.71788000	-1.15632400	1.57513700
H	-6.90725700	-1.47140000	-0.57716600
C	2.95598200	-1.26203100	-0.20876300
C	3.79016800	-1.49787100	0.88681600
C	3.52407600	-1.04394100	-1.46538100
C	5.17153300	-1.50904800	0.72680300
H	3.36226200	-1.69528300	1.86278800
C	4.90577700	-1.04196000	-1.62281800
H	2.86717300	-0.87005200	-2.30898400
C	5.73249100	-1.27566400	-0.52674100
H	5.81058600	-1.70420000	1.57979200
H	5.33815400	-0.86067400	-2.59983900
H	6.80921800	-1.28089100	-0.64887400
Li	-0.91522600	-2.26879300	-1.15816000

Zero-point correction=	0.335523 (Hartree/Particle)
Thermal correction to Energy=	0.358598
Thermal correction to Enthalpy=	0.359542
Thermal correction to Gibbs Free Energy=	0.280109
Sum of electronic and zero-point Energies=	-1479.501249

Sum of electronic and thermal Energies=	-1479.478174
Sum of electronic and thermal Enthalpies=	-1479.477230
Sum of electronic and thermal Free Energies=	-1479.556664

12Zd

S	-1.07170200	0.10081900	1.48288000
O	-1.79757300	-1.16400500	1.78663300
O	-1.33200800	1.21829100	2.39902100
C	0.60010400	-0.20430900	1.38236900
C	1.04091600	-1.24555000	0.57364600
C	-1.71424500	0.55389500	-0.16030000
C	-0.97615100	1.19759600	-1.06842100
H	-1.44209500	1.34547600	-2.04200900
O	0.27831900	-2.08685600	0.00821600
C	-3.09357600	0.08276200	-0.43787200
C	-3.35546400	-0.66678800	-1.58654200
C	-4.14326800	0.39191300	0.43279700
C	-4.65181400	-1.08719700	-1.87119200
H	-2.53820300	-0.92661400	-2.25054600
C	-5.43555500	-0.02967500	0.14704300
H	-3.94262100	0.96685000	1.33039600
C	-5.69361300	-0.76895700	-1.00607900
H	-4.84448800	-1.66807200	-2.76538200
H	-6.24382100	0.22045900	0.82381700
H	-6.70231600	-1.09784900	-1.22568300
C	0.39260600	1.73925700	-0.92050100
C	1.41143200	1.27368800	-1.75527600
C	0.67962600	2.71698300	0.03463200
C	2.71192900	1.73944700	-1.59936500
H	1.18923700	0.51919100	-2.50270100
C	1.97814400	3.19504000	0.17639500
H	-0.11344100	3.08346800	0.67709300
C	2.99855000	2.69881200	-0.63147600
H	3.50301600	1.34784000	-2.22855800
H	2.19425600	3.95022100	0.92294500
H	4.01235100	3.06204600	-0.51082700
C	2.51467400	-1.34433800	0.30257200
C	2.92829200	-2.00064700	-0.85792400
C	3.47420900	-0.77230900	1.14106600
C	4.27702900	-2.06078200	-1.19157400
H	2.17748600	-2.44758100	-1.49801900
C	4.82387700	-0.84239700	0.81438300
H	3.17269500	-0.28175700	2.05919300
C	5.22814000	-1.47890900	-0.35710100
H	4.58669500	-2.56037800	-2.10211700
H	5.56102200	-0.40114300	1.47483800

H	6.27988800	-1.52685100	-0.61399300
H	1.21777400	0.61421700	1.71248700
Li	-1.36171900	-2.69242400	0.69812000

Zero-point correction=	0.335551 (Hartree/Particle)
Thermal correction to Energy=	0.358500
Thermal correction to Enthalpy=	0.359444
Thermal correction to Gibbs Free Energy=	0.281435
Sum of electronic and zero-point Energies=	-1479.503552
Sum of electronic and thermal Energies=	-1479.480603
Sum of electronic and thermal Enthalpies=	-1479.479659
Sum of electronic and thermal Free Energies=	-1479.557668

12Ee

S	-0.13944800	-1.82992300	-0.31444200
O	-0.07123600	-2.54476500	0.99194000
O	0.25918300	-2.62394600	-1.48209500
C	-1.69619200	-1.18273200	-0.56412000
H	-1.96056900	-1.09493300	-1.60585700
C	-2.47549800	-0.71171700	0.48835000
C	1.07691200	-0.50217300	-0.16414000
C	0.64798700	0.76257500	-0.17646900
H	-0.41795300	0.92654700	-0.31631800
O	-2.12714300	-0.69044900	1.70449600
C	2.47859100	-0.98358800	-0.12607300
C	2.97261400	-1.71580900	0.95608400
C	3.32266900	-0.68686400	-1.20000200
C	4.30185100	-2.12740000	0.96971000
H	2.31664500	-1.95172500	1.78471000
C	4.64899400	-1.10092900	-1.18332900
H	2.93277000	-0.12401900	-2.04070300
C	5.14190400	-1.81967000	-0.09660400
H	4.68144300	-2.68772200	1.81582500
H	5.29707900	-0.86476200	-2.01886600
H	6.17641300	-2.14145500	-0.08301400
C	1.45808500	1.98812300	-0.05124900
C	0.95724700	3.16081100	-0.62954000
C	2.67550600	2.04539700	0.64029900
C	1.66895200	4.35258200	-0.55561700
H	0.00414700	3.13176600	-1.14672300
C	3.37863100	3.24057500	0.72539800
H	3.06665400	1.16014800	1.12564300
C	2.88416500	4.39465700	0.12107900
H	1.27106100	5.24765700	-1.01848900
H	4.31500400	3.27263400	1.26962900
H	3.43868400	5.32311200	0.18736900

C	-3.83270600	-0.15650200	0.15182000
C	-4.39227400	0.78625700	1.01674400
C	-4.55051600	-0.55589800	-0.97815700
C	-5.63847500	1.33992800	0.74510300
H	-3.83554300	1.08009300	1.89805600
C	-5.80312700	-0.01207900	-1.24253600
H	-4.14542500	-1.31088600	-1.64150500
C	-6.34707400	0.94135500	-0.38554600
H	-6.05860700	2.07963600	1.41637900
H	-6.35715200	-0.33701500	-2.11515400
H	-7.32133000	1.36699400	-0.59503800
Li	-0.97601800	-1.88847500	2.54439600

Zero-point correction= 0.335736 (Hartree/Particle)
 Thermal correction to Energy= 0.358874
 Thermal correction to Enthalpy= 0.359819
 Thermal correction to Gibbs Free Energy= 0.279875
 Sum of electronic and zero-point Energies= -1479.506874
 Sum of electronic and thermal Energies= -1479.483736
 Sum of electronic and thermal Enthalpies= -1479.482791
 Sum of electronic and thermal Free Energies= -1479.562735

12Ef

S	-0.30902400	-0.78595700	-1.98701200
O	-0.13137800	-2.24943500	-2.24418000
O	-0.12722600	0.05971500	-3.17277300
C	-1.80271300	-0.62698600	-1.20179700
H	-2.32131100	-1.56044200	-1.05950600
C	-2.18790800	0.62590400	-0.69186600
C	0.99131500	-0.33574300	-0.82016200
C	1.58363600	0.84769800	-1.00516700
H	1.28443800	1.41466700	-1.88185000
O	-1.55402800	1.68464500	-0.86116000
C	1.29530400	-1.34032900	0.22573800
C	0.36019100	-1.70522700	1.19883800
C	2.56605600	-1.92553500	0.24533200
C	0.69490700	-2.64121100	2.17306100
H	-0.61966800	-1.24240200	1.19720600
C	2.89743300	-2.85896700	1.22113500
H	3.29445600	-1.63234100	-0.50312400
C	1.96115100	-3.21970000	2.18736800
H	-0.03372800	-2.91223100	2.92795400
H	3.88639400	-3.30191100	1.22910000
H	2.21889900	-3.94489400	2.95002900
C	2.62199200	1.46825900	-0.16292100
C	2.71627700	1.26077000	1.21956100
C	3.53606700	2.33298700	-0.77703000

C	3.71601100	1.88263800	1.95697400
H	1.99568500	0.62747300	1.72193900
C	4.54515000	2.94280100	-0.04044100
H	3.45437700	2.52080700	-1.84224800
C	4.63956300	2.71650700	1.32953400
H	3.77134900	1.72081700	3.02696900
H	5.25058800	3.60062100	-0.53390300
H	5.41984800	3.19635300	1.90823200
C	-3.46315700	0.67495100	0.12171200
C	-4.12662500	1.89936300	0.22508900
C	-3.98492500	-0.43581900	0.78895000
C	-5.29903800	2.01003400	0.96395700
H	-3.70688000	2.75864500	-0.28375800
C	-5.15253800	-0.32445500	1.53870200
H	-3.47206900	-1.38958200	0.74487600
C	-5.81509600	0.89699300	1.62394800
H	-5.80957400	2.96390100	1.02858900
H	-5.54207500	-1.19079400	2.06043200
H	-6.72568800	0.98211700	2.20535300
Li	1.11402800	-3.62149500	-2.26743100

Zero-point correction=	0.334986 (Hartree/Particle)
Thermal correction to Energy=	0.358437
Thermal correction to Enthalpy=	0.359381
Thermal correction to Gibbs Free Energy=	0.278987
Sum of electronic and zero-point Energies=	-1479.488647
Sum of electronic and thermal Energies=	-1479.465197
Sum of electronic and thermal Enthalpies=	-1479.464252
Sum of electronic and thermal Free Energies=	-1479.544646

12Eg

S	-0.20594300	-0.68992800	-2.15710300
O	-0.15277300	-2.14617000	-2.50507700
O	0.08613100	0.19880300	-3.28712900
C	-1.69248100	-0.43166000	-1.37912000
H	-2.31796900	-1.30683000	-1.31377600
C	-1.93959100	0.79057700	-0.73076100
C	1.08459000	-0.43761900	-0.92581100
C	1.88576000	0.61678700	-1.09523500
H	1.71118500	1.21576100	-1.98478200
O	-1.20130600	1.79243000	-0.78901300
C	0.99418500	-1.34663500	0.24006400
C	0.33160000	-0.91245600	1.39090900
C	1.55637800	-2.62434300	0.20697400
C	0.24936000	-1.74224400	2.50407800
H	-0.10878400	0.07934600	1.40196400

C	1.47372600	-3.45265700	1.32276400
H	2.07256200	-2.95453600	-0.68768600
C	0.82209600	-3.01180400	2.47208800
H	-0.26073500	-1.39837700	3.39614300
H	1.92317200	-4.43840100	1.29733600
H	0.76160400	-3.65590500	3.34138100
C	2.95171700	1.11216100	-0.20851800
C	3.36164900	2.44061900	-0.38519200
C	3.58046500	0.34429100	0.78211600
C	4.34735300	2.99922000	0.41947300
H	2.89284000	3.03936700	-1.15862100
C	4.57364800	0.90129400	1.57833200
H	3.30820800	-0.69288100	0.92479200
C	4.95604600	2.22993000	1.40636900
H	4.64290100	4.03105900	0.27216400
H	5.05468800	0.29329200	2.33535400
H	5.72913900	2.65888600	2.03270800
C	-3.20028900	0.87621900	0.10016000
C	-3.80782500	2.12441700	0.24982300
C	-3.75663100	-0.23097000	0.74444500
C	-4.96518000	2.26120400	1.00794200
H	-3.35957300	2.98120200	-0.23900500
C	-4.90760100	-0.09329100	1.51550600
H	-3.27766200	-1.20031200	0.66591600
C	-5.51800600	1.15132600	1.64355300
H	-5.43548800	3.23264300	1.10671600
H	-5.32454600	-0.95670200	2.02075700
H	-6.41648000	1.25722800	2.24018900
Li	-0.81406300	-3.76423100	-1.88263100

Zero-point correction=	0.334527 (Hartree/Particle)
Thermal correction to Energy=	0.358286
Thermal correction to Enthalpy=	0.359230
Thermal correction to Gibbs Free Energy=	0.276738
Sum of electronic and zero-point Energies=	-1479.489392
Sum of electronic and thermal Energies=	-1479.465632
Sum of electronic and thermal Enthalpies=	-1479.464688
Sum of electronic and thermal Free Energies=	-1479.547180

12Eh

S	-0.12584900	2.10852100	-0.78620200
O	-0.02830700	2.50050300	-2.22710700
O	0.27614000	3.28529500	0.04172800
C	-1.66114200	1.47375100	-0.50186800
H	-2.30008000	1.47515400	-1.36967900
C	-1.90247200	0.81573500	0.71937700

C	1.07799000	0.80700600	-0.47939400
C	2.06961900	1.07423000	0.37357800
H	2.05604100	2.04980900	0.85169700
O	-1.12261800	0.83671800	1.68957600
C	0.74528100	-0.47732000	-1.13744700
C	0.32820200	-1.55017800	-0.34466000
C	0.81933900	-0.62677100	-2.52323700
C	0.00654200	-2.76718400	-0.93365400
H	0.25432200	-1.41317100	0.72850400
C	0.49823700	-1.84793800	-3.10877000
H	1.13213700	0.21217200	-3.13396100
C	0.09377400	-2.91857100	-2.31611600
H	-0.31617800	-3.59620600	-0.31499700
H	0.56477300	-1.96300200	-4.18410300
H	-0.15635300	-3.86812000	-2.77438200
C	3.16871000	0.18301700	0.78013900
C	3.64590600	-0.87352900	-0.00774400
C	3.77796100	0.42798900	2.01706900
C	4.68846800	-1.67156000	0.44609200
H	3.21306500	-1.06439400	-0.98149600
C	4.81262200	-0.37934000	2.47508200
H	3.42713200	1.25457900	2.62544400
C	5.26922900	-1.43403200	1.69043200
H	5.05230200	-2.48076200	-0.17582600
H	5.26441400	-0.18167800	3.43969000
H	6.07923200	-2.06253600	2.04085700
C	-3.19062400	0.03953000	0.84201600
C	-3.73204800	-0.14485100	2.11578000
C	-3.83426500	-0.52596500	-0.26051000
C	-4.91084300	-0.86217400	2.28424000
H	-3.21459000	0.28345800	2.96600500
C	-5.00785800	-1.25495500	-0.09170600
H	-3.40650200	-0.42098100	-1.25100300
C	-5.55143500	-1.41944900	1.17954900
H	-5.32923300	-0.99042600	3.27574100
H	-5.49440600	-1.69977000	-0.95180300
H	-6.46736900	-1.98396100	1.30951700
Li	0.46199900	4.44291200	-1.62134300

Zero-point correction=	0.334159 (Hartree/Particle)
Thermal correction to Energy=	0.358019
Thermal correction to Enthalpy=	0.358963
Thermal correction to Gibbs Free Energy=	0.276301
Sum of electronic and zero-point Energies=	-1479.490512
Sum of electronic and thermal Energies=	-1479.466652
Sum of electronic and thermal Enthalpies=	-1479.465708
Sum of electronic and thermal Free Energies=	-1479.548370

Ring opened products 7:

trans-Diphenylethenyl sulfone 7E

C	2.74167800	4.05812900	-0.18865600
C	1.75370000	3.13828400	-0.51887400
C	2.05531100	1.77607300	-0.63808600
C	3.38078800	1.35700000	-0.45986500
C	4.36913300	2.28074300	-0.14682500
C	4.05216900	3.63011500	-0.00019800
H	2.49032300	5.10699000	-0.08820600
H	0.73449900	3.47280700	-0.67932700
H	3.64351000	0.31393600	-0.58281900
H	5.39220300	1.94758500	-0.02030900
H	4.82695600	4.34524300	0.24918200
C	0.95264900	0.86440500	-0.97821500
H	0.11169400	1.32194400	-1.49338800
C	0.86490200	-0.44408000	-0.71273700
C	1.77746100	-1.28964000	0.09159000
C	2.47205200	-2.35826000	-0.48037700
C	1.95197100	-0.99248000	1.44689400
C	3.34986700	-3.10879900	0.29493400
H	2.32735000	-2.59064700	-1.52821000
C	2.82950300	-1.74676100	2.21668200
H	1.39336100	-0.17228300	1.88294700
C	3.53151200	-2.80322900	1.64105600
H	3.89324600	-3.93158700	-0.15381800
H	2.96350200	-1.51184900	3.26577400
H	4.21620500	-3.38998200	2.24184200
C	-1.50783200	-1.67137600	0.21702200
H	-2.30597400	-2.34129900	-0.10034300
H	-0.79709200	-2.20662600	0.84747400
C	-1.98091500	-0.41834500	0.94155000
O	-1.22623700	0.11496100	1.72483800
C	-3.34510800	0.11450300	0.67531600
C	-4.13936100	-0.34733300	-0.37757100
C	-3.82654900	1.12436100	1.51592600
C	-5.40104700	0.19855100	-0.58642500
H	-3.77701200	-1.10826400	-1.05654800
C	-5.08947600	1.65902600	1.31160200
H	-3.19980500	1.47381100	2.32720800
C	-5.87756600	1.19625600	0.25818500
H	-6.01044500	-0.15508300	-1.40877600
H	-5.46194000	2.43509600	1.96889500
H	-6.86372300	1.61517600	0.09652200

S	-0.61533200	-1.25960100	-1.30004600
O	-0.24683100	-2.52587200	-1.92958000
O	-1.42950600	-0.31086300	-2.05837700

Zero-point correction= 0.346472 (Hartree/Particle)

Thermal correction to Energy= 0.368651

Thermal correction to Enthalpy= 0.369595

Thermal correction to Gibbs Free Energy= 0.291314

Sum of electronic and zero-point Energies= -1472.470476

Sum of electronic and thermal Energies= -1472.448297

Sum of electronic and thermal Enthalpies= -1472.447353

Sum of electronic and thermal Free Energies= -1472.525635

***cis*-Diphenylethenyl sulfone 7Z**

C	4.51180500	-1.08752700	-1.63105700
C	3.30484000	-0.39884100	-1.63039600
C	2.98763900	0.46871400	-0.57874900
C	3.91085300	0.66763800	0.44947700
C	5.12606900	-0.00992100	0.43478500
C	5.42532500	-0.89369800	-0.59744700
H	4.74097500	-1.77022800	-2.44046400
H	2.59007700	-0.54676400	-2.43211500
H	3.67493400	1.34954700	1.25535600
H	5.83853600	0.15288900	1.23458700
H	6.37006400	-1.42424300	-0.60139300
C	1.70034500	1.19915700	-0.65161600
H	1.57811900	1.82001700	-1.53889000
C	0.63791000	1.16766400	0.15921400
C	-0.64095800	1.85059800	-0.16030900
C	-1.25532500	2.71430000	0.75137200
C	-1.23435800	1.62862700	-1.40570700
C	-2.43869500	3.35696300	0.41145300
H	-0.80337700	2.88379800	1.72105100
C	-2.42153300	2.27204300	-1.74166500
H	-0.77021800	0.93532800	-2.09949300
C	-3.02476400	3.13613900	-0.83386300
H	-2.90539600	4.03139000	1.11920000
H	-2.87676300	2.09019200	-2.70792300
H	-3.95089100	3.63540300	-1.09265100
C	0.56893000	-1.58726800	0.74432400
H	1.58550500	-1.74329000	0.38403500
H	0.33061400	-2.29416300	1.53996700
C	-0.38347700	-1.63842400	-0.44653600
O	0.09163000	-1.55020700	-1.55792600
C	-1.84980000	-1.76469700	-0.22958700
C	-2.40751300	-2.00382300	1.02878400
C	-2.68610600	-1.63087800	-1.34472900

C	-3.78701900	-2.11287300	1.16722300
H	-1.78239200	-2.09487800	1.90676600
C	-4.06086000	-1.73192700	-1.20236100
H	-2.24059400	-1.44031800	-2.31358700
C	-4.61222000	-1.97531900	0.05591100
H	-4.21594500	-2.30076400	2.14362900
H	-4.70494100	-1.62155100	-2.06612500
H	-5.68697500	-2.05600200	0.16834900
S	0.58468200	0.03234700	1.56106900
O	-0.69164400	0.21445100	2.24588300
O	1.80592000	0.10028200	2.35597500

Zero-point correction= 0.346180 (Hartree/Particle)

Thermal correction to Energy= 0.368287

Thermal correction to Enthalpy= 0.369231

Thermal correction to Gibbs Free Energy= 0.292120

Sum of electronic and zero-point Energies= -1472.461311

Sum of electronic and thermal Energies= -1472.439205

Sum of electronic and thermal Enthalpies= -1472.438260

Sum of electronic and thermal Free Energies= -1472.515372