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Mechanistic investigation in the [1,4] and [1,2] Wittig rearrangement reactions : A DFT study

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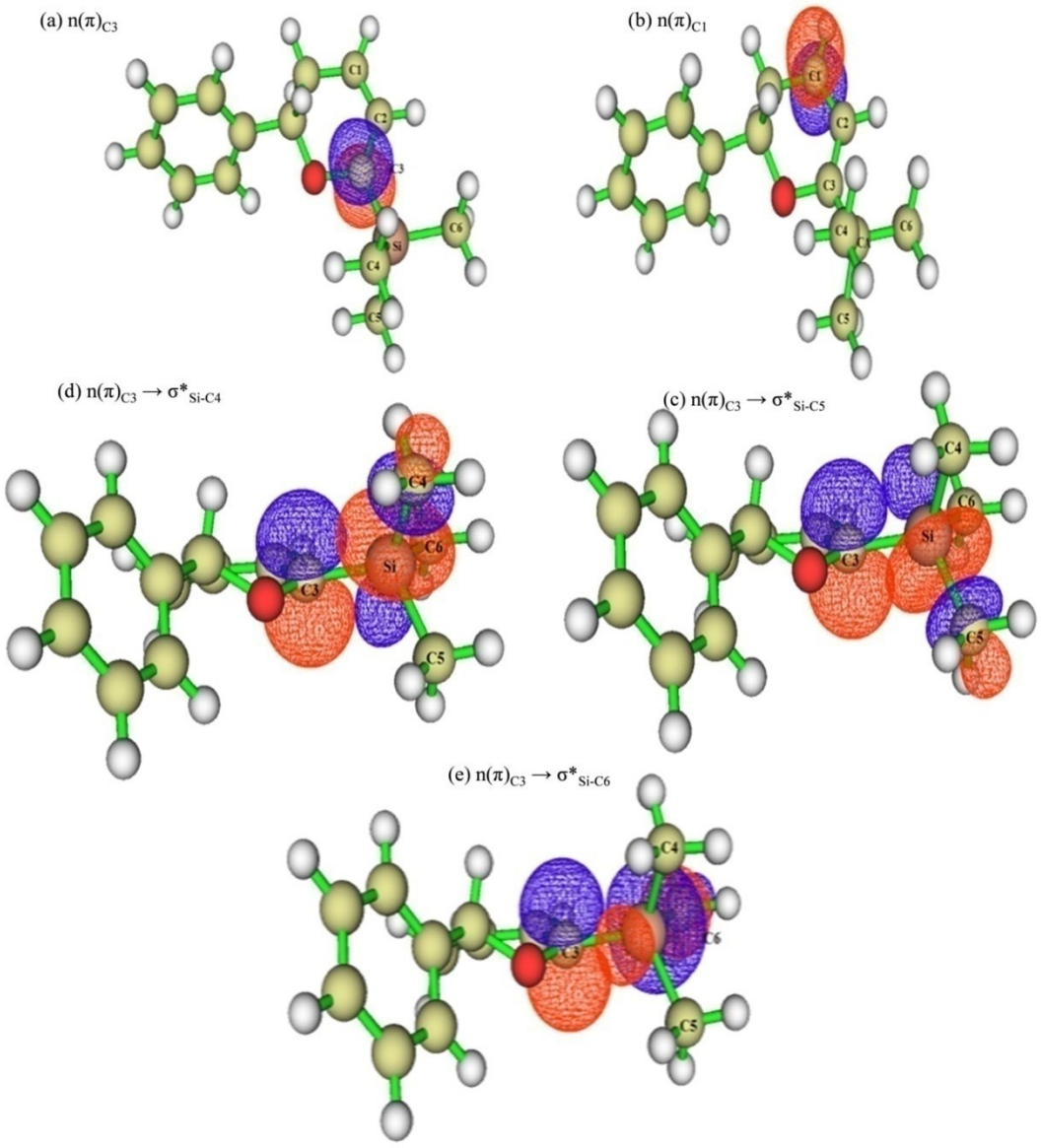


Figure S1 Selected Natural Bond orbital interactions for the anionic intermediate structure of conformer 1b. The first orbital plot shows the lone pair at the C^3 atom of the Silyl substituted structure. NBO for the equivalent *t*-butyl substituted structure with the lone pair on the C^1 carbon can be seen in Figure b. Interactions with the various anti-bonding orbitals on C4, C5 and C6 for the Silyl substituted structure can be seen in d-e

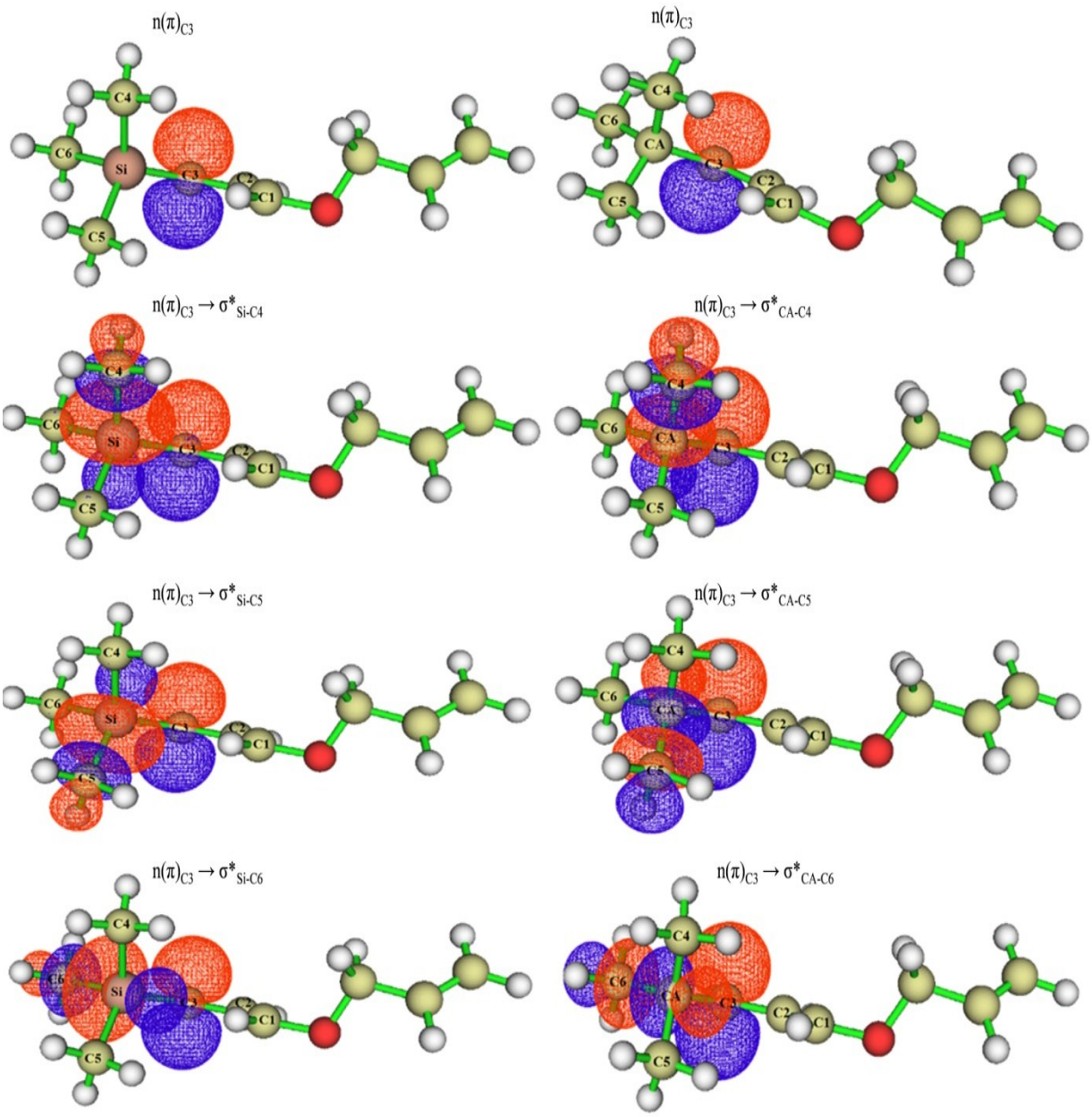


Figure S2 Selected Natural Bond orbital interactions for Molecules 4a and 4aC. The first two orbital plots shows the corresponding lone pair NBOs at the C^3 atom for the anionic intermediates of 4a and 4aC. Interactions with the various anti-bonding orbitals on C4, C5 and C6 have been shown in the rest of the plots.

The associated donor-acceptor perturbation energies and other significant factors for selected anionic and Lithiated intermediates of the molecule shown in Table 4 have been tabulated in Table S1 and Table S2. Selected NBO plots for the α and γ-substituted anions have also been shown in FiguresS1 and S2. It is evident from Table S1 that the perturbation energies arising from the donation of electron density into the antibonding orbitals of the Si-C groups are much higher

compared to their C-C equivalents for the α as well as γ substituted intermediates. This may be understood by analyzing the equation for second order perturbation energy calculations in the NBO basis (1).

$$E(2) = -n_\sigma \frac{\langle \sigma | F | \sigma^* \rangle^2}{\varepsilon_{\sigma^*} - \varepsilon_\sigma} = -n_\sigma \frac{F_{ij}^2}{\Delta E} \qquad (1)$$

The second order perturbation energy from NBO analysis (E(2)) depends on the square of the Fock matrix element, F_{ij} which reflects the extent of overlap of the interacting orbitals i and j, as well as their natural bond orbital energies (ε_{σ^*}, ε_σ). The values of these elements for the selected anionic and Lithiated intermediates of the molecules under consideration are given in Table S1. The NBO occupancies of the donor orbital (n_σ) have been included in Table S2.

A comparison of these elements for α and γ, Silyl and t-butyl substituted, anionic intermediates listed in Table S1 shows that the perturbation energies arising from the donor-acceptor interactions of the anion at C^3 with the Me_3-Si orbital are much larger than those for the equivalent Me_3-C orbitals. The orbital energy gaps for the silylated molecules are relatively lower and they show greater overlap densities in comparison with their carbon analogues. Also, the NBO occupancies for the lone pair orbital (n_σTable S2) are also higher (~1.5) for the silylated analogues and relatively lower (~1.4) for the t-butyl substituted ones. Thus, in addition to the stabilization offered by the adjacent C^1-C^2 π bond of the allylic complex, negative hyperconjugation by the TMS groups plays a crucial role in the stabilization of the deprotonated intermediates of the Wittig reactants.

The lower orbital energy differences for the silylated analogues can in turn be attributed to the polarization coefficients of the Si and C atoms. Si being more electropositive has a significantly larger polarization coefficient, causing an increase in the polarity of the σ bond and a consequent lowering in the orbital energy difference. These have also been shown in Table S2.

Table S1: Significant NBO second-order perturbation energies (E(2) kcal.mol^{-1}) and occupancy numbers, Fock matrix elements and orbital energy differences for selected anionic and Lithiated forms of the molecules depicted in Table 4 of the main manuscript.

α-Substitution							
Lithiated Intermediates of 2-silyl-6-aryl-5,6-dihydro-*2H*-pyran							
	1b				**2a**		
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	9.46	0.07	0.48	$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	10.43	0.074	0.48
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	5.08	0.052	0.48	$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	3.29	0.042	0.48
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	-	-	-	$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	0.91	0.022	0.48
Anionic Intermediates of 2-silyl-6-aryl-5,6-dihydro-*2H*-pyran							
	1				**2**		
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	13.26	0.075	0.4	$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	14.08	0.078	0.4
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	12.25	0.073	0.4	$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	11.79	0.071	0.4
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	-	-	-	$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	-	-	-
Silyl substitution	E(2) kcal mol-1	F_{ij}	ε_j-ε_i	**t-Butyl Substitution**	E(2) kcal mol^{-1}	F_{ij}	ε_j-ε_i
	3a[a]				**3aC**		
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	16.26	0.104	0.67	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C4}$	10.47	0.076	0.52
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	5.74	0.054	0.51	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C5}$	3.83	0.047	0.53
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	2.72	0.036	0.48	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C6}$	0.78	0.021	0.54
γ-Substitution							

Silyl substituted intermediates	E(2) kcal mol^{-1}	F_{ij}	ε_j-ε_i	**t-Butyl substituted intermediates**	E(2) kcal mol^{-1}	F_{ij}	ε_j-ε_i
	4a				**4aC**		
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	14.56	0.077	0.41	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C4}$	7.99	0.066	0.52
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	14.11	0.076	0.41	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C5}$	7.68	0.067	0.52
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	-	-	-	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C6}$	-	-	-
	4b						
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	18.98	0.087	0.41				
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	7.8	0.057	0.41				
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	1.59	0.026	0.4				
	5a				**5aC**		
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	14.61	0.077	0.41	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C4}$	8.08	0.067	0.52
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	14.14	0.076	0.41	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C5}$	7.61	0.065	0.52
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	-	-	-	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C6}$	-	-	-
	5b				**5bC**		
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	14.7	0.078	0.41	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C4}$	8	0.67	0.52
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	13.88	0.075	0.41	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C5}$	7.68	0.066	0.52
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	-	-	-	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C6}$	-	-	-
	6a				**6aC**		
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	14.39	0.077	0.41	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C4}$	7.94	0.067	0.52
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	13.62	0.075	0.41	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C5}$	7.53	0.065	0.52

$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	-	-	-	$n(\pi)_{C3} \rightarrow \sigma^*_{CA-C6}$	-	-	-
6b							
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C4}$	17.92	0.084	0.41				
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C5}$	9.46	0.063	0.41				
$n(\pi)_{C3} \rightarrow \sigma^*_{Si-C6}$	2.46	0.032	0.42				

[a]The natural Lewis structure for the Silyl substituted anionic intermediate of 3a, shows a double bond between the Si and C^3 atoms instead of a lone pair at C^3. The calculated (E2) energies for this system are for the interactions of this double bond with the σ* orbitals of the Si-Me bonds.

Table S2 NBO energies (E), occupancies (Occ.) and polarization coefficients (*c*) for selected anionic and Lithiated intermediates of the molecules shown in Table 4 of the main manuscript.

α-Substitution									
Silyl Orbital	NBO (E)	NBO Occ.	*c*(Si)	*c*(C')	***t*-Butyl Orbital**	NBO (E)	NBO Occ.	*c*(CA)	*c*(C')
		3a					**3aC**		
$n(\pi)_{C3}$	0.00005	1.56433	0.2423	0.9702	$n(\pi)_{C3}$	0.04597	1.43823	-	-
σ^*_{Si-C4}	0.67456	0.05947	0.8966	-0.4427	σ^*_{CA-C4}	0.04312	0.04312	-0.7028	0.7114
σ^*_{Si-C5}	0.51122	0.04063	0.8709	-0.4915	σ^*_{CA-C5}	0.57266	0.02538	-0.7017	0.7124
σ^*_{Si-C6}	0.47596	0.03987	0.8637	-0.5041	σ^*_{CA-C6}	0.58334	0.02031	-0.6984	0.7157
Lithiated Intermediates									
		1b					**2a**		
$n(\pi)_{C3}$	-0.16206	1.40143	-	-	$n(\pi)_{C3}$	1.37979	1.37979		
σ^*_{Si-C4}	0.31462	0.05538	0.8528	-0.5223	σ^*_{Si-C4}	0.32215	0.05915	-0.8516	0.5242
σ^*_{Si-C5}	0.31324	0.04842	0.8545	-0.5194	σ^*_{Si-C5}	0.31927	0.04346	-0.8543	0.5198
σ^*_{Si-C6}	0.33581	0.04066	0.8645	-0.5026	σ^*_{Si-C6}	0.32012	03382	-0.8548	0.5190
Anionic Intermediates									
		1					**2**		

$n(\pi)_{C3}$	0.0286	1.40183			$n(\pi)_{C3}$	0.02865	1.41786		
σ^*_{Si-C4}	0.42994	0.08606	-0.8609	0.5087	σ^*_{Si-C4}	0.43218	0.08348	0.8606	0.5093
σ^*_{Si-C5}	0.42920	0.07947	-0.8610	0.5087	σ^*_{Si-C5}	0.43287	0.08237	0.8607	-0.5092
σ^*_{Si-C6}	0.43741	0.03057	-0.8600	0.5103	σ^*_{Si-C6}	0.43901	0.03213	0.8606	-0.5093

γ-Substitution									
Silyl Orbital	NBO (E)	NBO Occ.	*c*(Si)	*c*(C')	***t*-Butyl Orbital**	NBO (E)	NBO Occ.	*c*(CA)	*c*(C')
		4a					**4aC**		
$n(\pi)_{C3}$	0.03444	1.52297	-	-	$n(\pi)_{C3}$	0.05458	1.45288		
σ^*_{Si-C4}	0.44250	0.08121	0.8628	-0.5056	σ^*_{CA-C4}	0.57793	0.03433	-0.7018	0.7124
σ^*_{Si-C5}	0.44227	0.07904	0.8628	-0.5055	σ^*_{CA-C5}	0.57877	0.03371	-0.7017	0.7125
σ^*_{Si-C6}	0.45023	0.02926	0.8630	-0.5052	σ^*_{CA-C6}	0.58661	0.01917	-0.7035	0.7107
		4b							
$n(\pi)_{C3}$	0.03185	1.51296							
σ^*_{Si-C4}	0.43435	0.10429	0.8642	-0.5031					
σ^*_{Si-C5}	0.44054	0.06271	0.8637	-0.5039					
σ^*_{Si-C6}	0.44192	0.03757	0.8628	-0.5055					
		5a					**5aC**		
$n(\pi)_{C3}$	0.03436	1.52262	-	-	$n(\pi)_{C3}$	0.05433	1.45275	-	-
σ^*_{Si-C4}	0.44205	0.08233	0.8627	-0.5057	σ^*_{CA-C4}	0.57760	0.03434	0.7124	-0.7017
σ^*_{Si-C5}	0.44252	0.07758	0.8628	-0.5056	σ^*_{CA-C5}	0.57844	0.03375	0.7124	-0.7017
σ^*_{Si-C6}	0.45016	0.02935	0.8630	-0.5052	σ^*_{CA-C6}	0.58639	0.01912	0.7107	-0.7035
		5b					**5bC**		

$n(\pi)_{C3}$	0.03512	1.52438	-	-	$n(\pi)_{C3}$	0.05515	1.45494	-	-
σ^*_{Si-C4}	0.44308	0.08116	0.8628	-0.5056	σ^*_{CA-C4}	0.57839	0.03457	-0.7018	0.7124
σ^*_{Si-C5}	0.44283	0.07968	0.8629	-0.5053	σ^*_{CA-C5}	0.57920	0.03362	-0.7017	0.7124
σ^*_{Si-C6}	0.45082	0.02928	0.8630	-0.5051	σ^*_{CA-C6}	0.58674	0.01912	-0.7036	0.7106
		6a					**6aC**		
$n(\pi)_{C3}$	0.03157	1.51377	-	-	$n(\pi)_{C3}$	0.05136	1.44234	-	-
σ^*_{Si-C4}	0.44034	0.07998	0.8624	-0.5062	σ^*_{CA-C4}	0.57561	0.03392	-0.7015	0.7127
σ^*_{Si-C5}	0.44035	0.07627	0.8625	-0.5061	σ^*_{CA-C5}	0.57601	0.03328	-0.7015	0.7127
σ^*_{Si-C6}	0.44792	0.02933	0.8627	-0.5056	σ^*_{CA-C6}	0.58356	0.01911	-0.7033	0.7109
		6b							
$n(\pi)_{C3}$	0.02844	1.51917	-	-					
σ^*_{Si-C4}	0.43390	0.10288	0.8642	-0.5031					
σ^*_{Si-C5}	0.43881	0.06218	0.8623	-0.5064					
σ^*_{Si-C6}	0.44800	0.04151	0.8630	-0.5052					

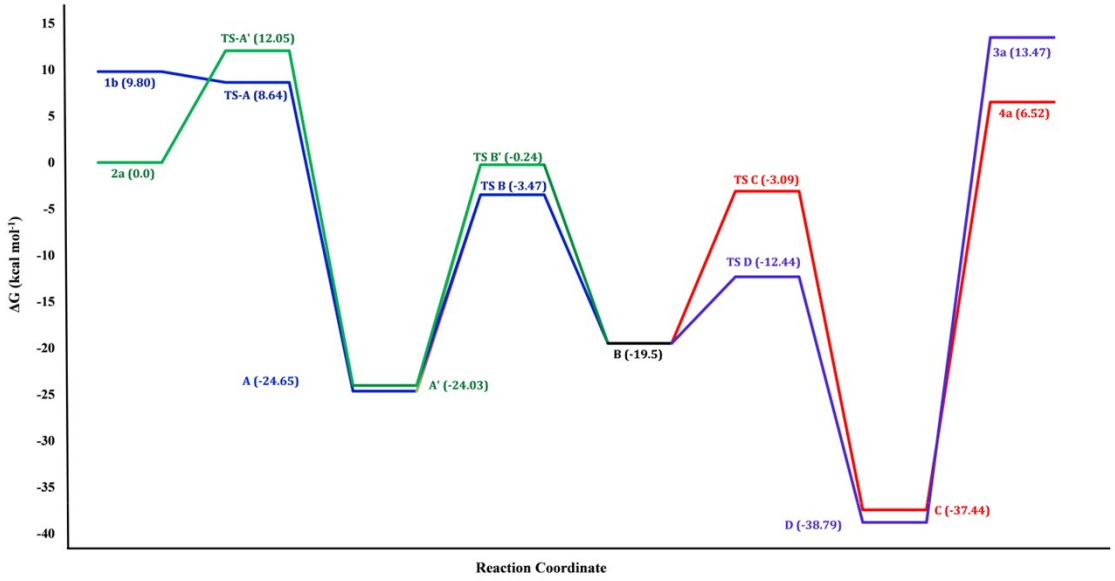


Figure S3: Plot of Change in Gibbs free energy values of the various stationary points along the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism reaction coordinate in the gas phase at a temperature of 195 K in kcal.mol^{-1}.

The energy profile plot using free energies of different transition states and intermediates has been made in the gas phase reaction condition qnd shown in Figure S3. The gas phase study aids in highlighting few interesting aspects of the mechanism. In contrast to the THF solvent reaction environment, in the gas phase, the conformer **1b** turns out to be ~ 10 kcal.mol^{-1} higher in energy than the **2a** conformer. The lower free energy value for **2a** in the gas phase, as discussed in section 3.2.1 of the main manuscript, is attributed to the increase in entropic contribution owing to the two pseudo-axial, bulky substituents. As may be seen, the deprotonation for the conformer **1b** does not have a positive barrier to the transition state **TS-A**, while, the conformer **2a** needs to overcome a barrier of ~ 12 kcal.mol^{-1} for the transition state **TS-A'**. The two conformers **1b** and **2a**, thereby, result respectively in to the intermediates **A** and **A'**, marginally differing in energy (0.62 kcal.mol^{-1}). Further, the Gas phase mechanistic pathway differs from the one in the solvent phase for the step of C-O bond cleavage. The C-O bond cleavage step initiated from the two intermediates **A** and **A'** undergoes two different transition states **TS-B** and **TS-B'**, respectively, unlike the solvent phase, where only one transition state **TS-Bs** is observed.

Table S3 Second-order perturbation energies (E(2) kcal mol^{-1}) for the donor-acceptor interactions of selected anionic intermediates for the Silyl substituted molecules listed in Table 4 along with the value of their respective dihedral angles Shown in Figure 9 of the main manuscript.

Anionic Intermediate	E(2) kcal mo^{l-1}	φ C^4-Si-C^3-C^2	E(2) kcal mo^{l-1}	φ C^5-Si-C^3-C^2
1-an	13.26	116.7[a]	11.79	123.9[a]
2-an	14.08	114.9[a]	12.25	126.3[a]
3a	16.26	89.5	5.74	152.5[a]
4a	14.56	61.4	14.11	59.41
4b	18.98	101.2	7.8	40.4
5a	14.61	61.1	14.14	59.4
5b	14.7	61.1	13.88	59.4
6a	14.39	61.6	13.62	58.9
6b	17.92	89.35	9.46	34.3

[a] For the α-substituted molecules, the listed dihedral angle values of φ C^4-Si-C^3-C^2 and φ C^5-Si-C^3-C^{2}used for plotting Figure 9 have been subtracted from 180 for the sake of consistency with the γ-substituted ones

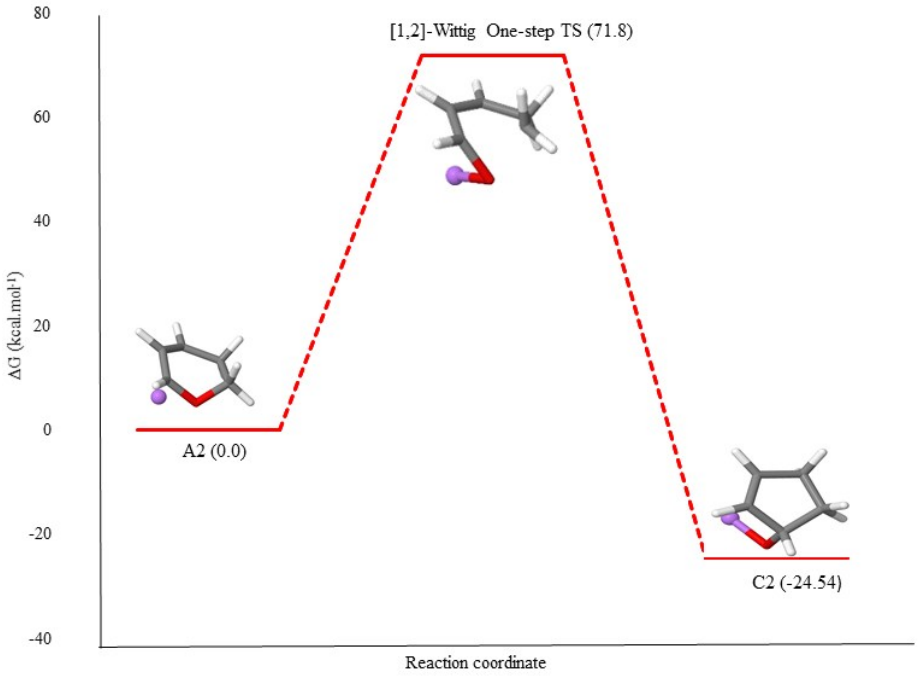


Figure S4 Gibbs free energy profile for the symmetry forbidden [1,2]-Wittig one-step transition state for the 5,6-dihydro-2H-pyran mechanism at 298.15 K in the gas phase.

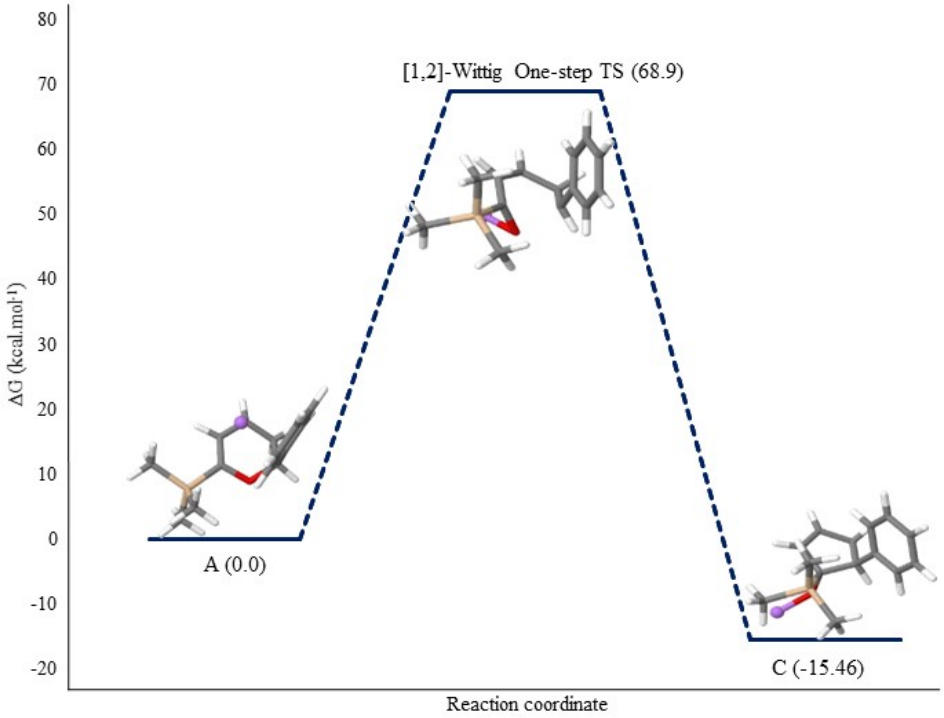


Figure S5 Gibbs free energy profile for the symmetry forbidden [1,2]-Wittig one-step transition state of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism at 298.15 K in the gas phase.

Effect of explicit solvent molecules on the reaction profile.

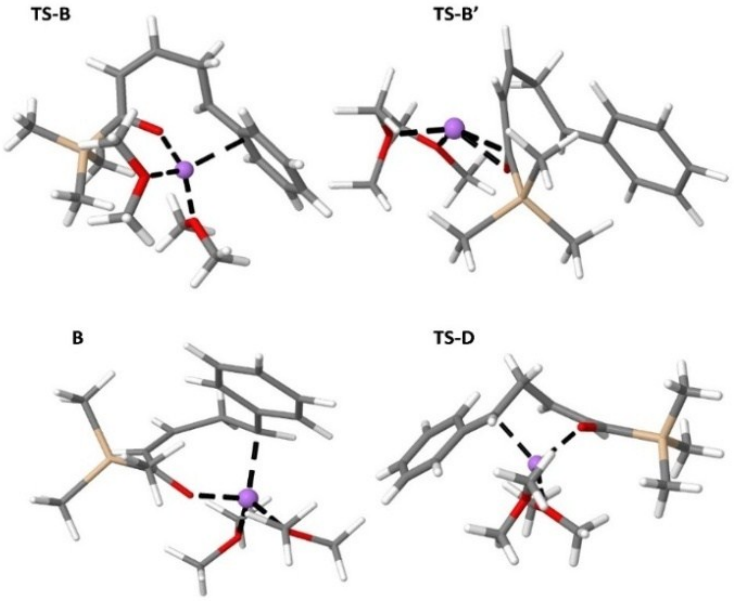


Figure S6. Selected three-dimensional structures of the intermediates and the transition states showing the Li counter-ion in coordination with two molecules of DME with implicit THF solvation.

The Reaction profile for the Wittig rearrangement reaction of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran molecule has further been explored by considering Dimethyl ether molecules representing the neighboring solvent molecules surrounding the lithium cation. Thus, the involved intermediate and transition state geometries of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran system have been re-optimized by including a solvation sphere of two dimethyl ether molecules (DME) around the Lithium counter-ion.[4e,44-47] Calculations involving more than two DME molecules in the solvation sphere around Lithium led to unstable structures. Therefore, the analysis of the study involving explicit solvent molecules has been carried out with a Tetracoordinated-Li system. This observation is in line with previous studies.[45,46]

The optimized geometries of some of the disolvated Li species studied have been shown in Figure S6. The Gibbs free energy profile starting from the **A** and **A**' intermediates obtained after deprotonation step as discussed in the previous section, is shown in Figure S7. As with the earlier reaction profiles, the [1,2]-Wittig rearrangement reaction once again turns out to be the pathway with higher activation energy than that the [1,4] sigmatropic rearrangement. The incorporation of the two DME molecules contribute in slightly lowering the activation energies for all the transition

states along these pathways. As observed earlier in case of gas phase energy profile, explicit solvent molecules show presence of two transition states **TS-B** and **TS-B'** located for homolytic C-O dissociation step of the mechanism, as seen in Figures S6 and S7.

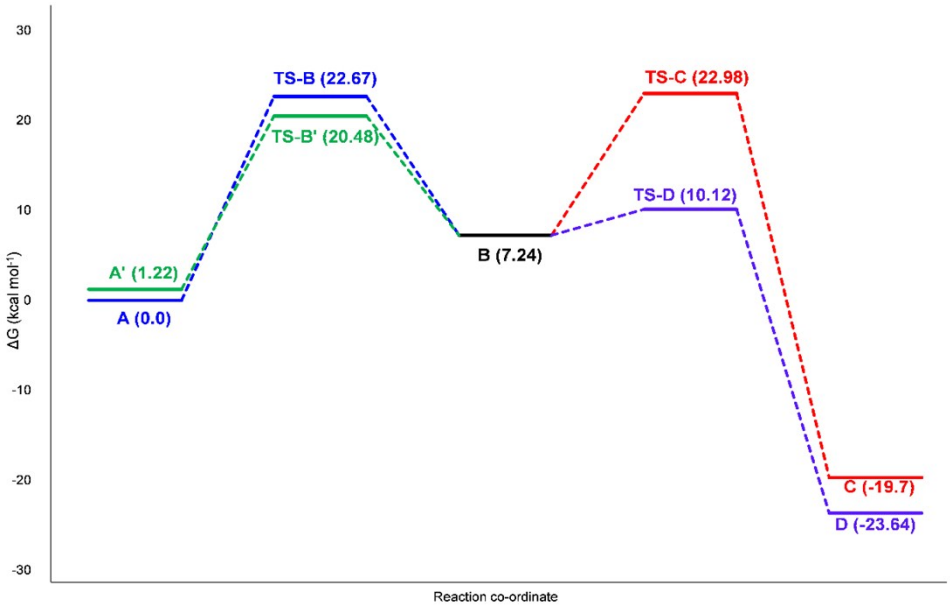


Figure S7. Relative Gibbs free energy values for the Lithiated intermediates and transition structures of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran model reaction in the presence of two molecules of dimethyl ether in THF.

The two transition states, once again differ with respect to the position of the Li cation in the molecular plane defined by the pyran ring. This is in contrast with the single transition state geometry obtained in the implicit solvent SCRF calculations, where the Li ion is observed to shift during the optimization procedure. The spatial restrictions and the rigidity imposed on the cation by the two dimethyl ether molecules may account for the absence of this phenomenon and the two resulting transition states for the C-O bond dissociation. Both of these transition states, however, still possess the highest activation energies along this profile and therefore, the C-O bond cleavage step is still the rate determining step for this reaction.

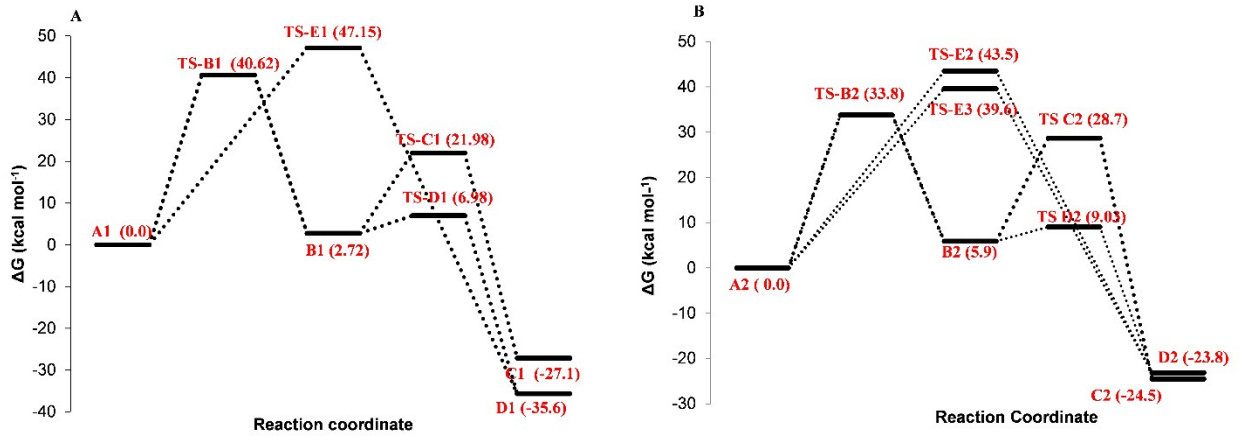


Figure S8: Mechanistic profile for the A) [1,2] and [1,4] Wittig rearrangements of 3-methoxypropene model system and B) 5,6-(2H)-dihydropyran model system at the 6-31+G(d,p) level of theory. Energies in parentheses are relative zero point corrected free energy values for with respected to the lithiated intermediate of each reactant.

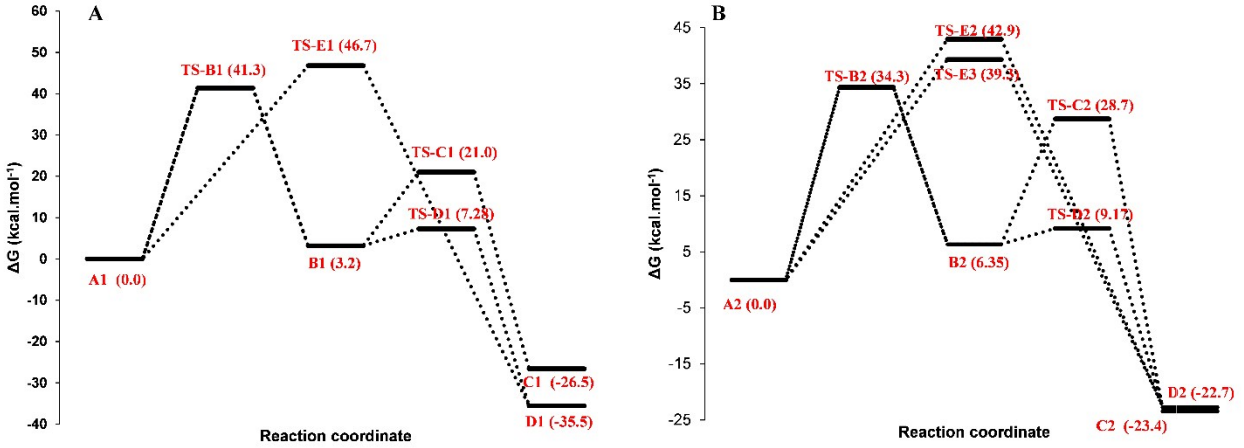


Figure S9: Mechanistic profile for the A) [1,2] and [1,4] Wittig rearrangements of 3-methoxypropene model system and B) 5,6-(2H)-dihydropyran model system at the M06-2X/cc-pVTZ level of theory. Energies in parentheses are relative zero point corrected free energy values for with respected to the lithiated intermediate of each reactant.

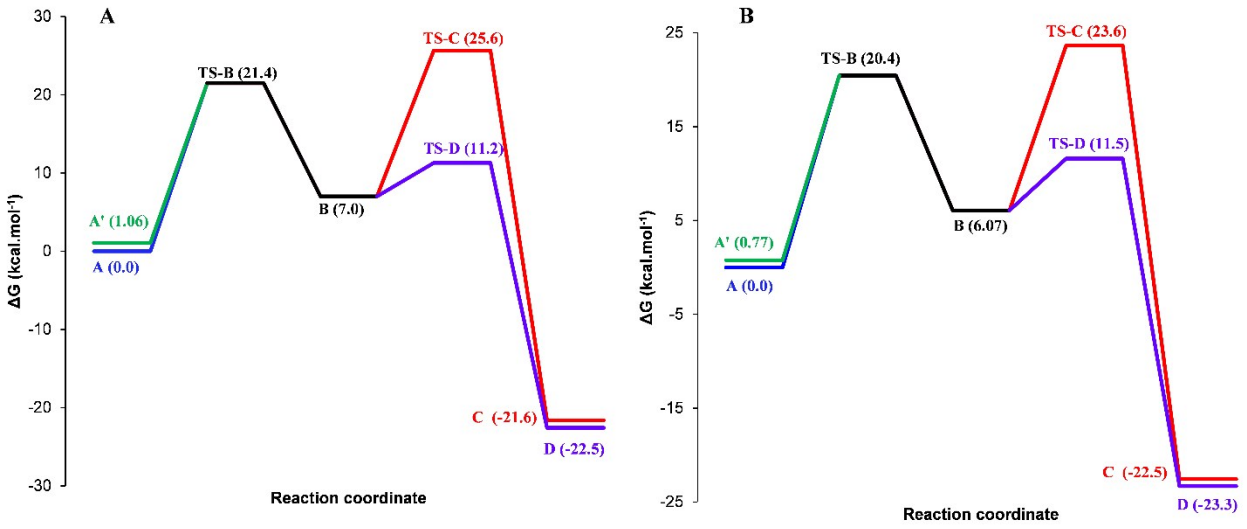


Figure S10: Plots of Change in Gibbs free energy values of the various stationary points along the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism reaction coordinate in THF solvent at a temperature of 195 K in kcal.mol^{-1} A) At the M062x/cc-pVTZ level of theory B) At the 6-311++G(d,p) level of theory.

1. Energies and Cartesian coordinates of M062x/6-31+G(d,p) optimized geometries for stationary points of the 3-methoxypropene mechanism at 298.15 K

A1			
C	1.59912	0.88270	0.02604
H	0.84699	1.66521	-0.05786
H	2.60126	1.22418	0.24764
C	1.21972	-0.41911	0.41796
H	1.98342	-1.07632	0.83301
C	0.01047	-1.03006	0.15125
H	-0.29066	-2.03002	0.43194
O	-0.96747	-0.24782	-0.51342
C	-1.74291	0.58057	0.35048
H	-1.09013	1.17946	0.99368
H	-2.39190	-0.04541	0.97098
H	-2.35202	1.23173	-0.28066
Li	0.63815	-0.08363	-1.56860

Electronic Energy = -239.249172750
Zero-point corrected electronic energy=-239.145706
Zero-point corrected Gibbs free energy=-239.17512

B1			
C	0.40871	1.50292	0.00015
H	-0.58131	1.03996	0.00030
H	0.45283	2.58783	0.00014
C	1.53941	0.78357	-0.00007
H	2.51667	1.25812	-0.00024
C	1.54005	-0.68557	-0.00011
H	2.52896	-1.17407	-0.00035
O	0.54514	-1.39817	0.00009
C	-2.80390	0.09113	-0.00009
H	-2.79828	0.75631	-0.88058
H	-3.79838	-0.38072	-0.00081
H	-2.79935	0.75617	0.88049
Li	-1.32927	-1.27018	0.00034

Electronic Energy = -239.235764998
Zero-point corrected electronic energy=-239.137654
Zero-point corrected Gibbs free energy=-239.170784

C1			
C	1.98007	0.12184	0.24697
H	1.76750	1.15796	0.49414
H	2.99154	-0.24408	0.39254

D1			
C	-1.06885	0.39148	-0.51844
H	-0.82768	-0.14003	-1.46317
H	-1.73915	1.19882	-0.83021

C	1.00972	-0.65918	-0.22271
H	1.22642	-1.69910	-0.47418
C	-0.42425	-0.21833	-0.43907
H	-0.63666	-0.40534	-1.51320
O	-0.64414	1.09471	-0.12709
C	-1.35582	-1.14233	0.36365
H	-1.20564	-2.19847	0.11228
H	-2.39727	-0.87763	0.15805
H	-1.16437	-1.00458	1.43318
Li	-0.89556	2.63384	0.24030

Electronic Energy = -239.290750225
Zero-point corrected electronic energy=-239.187206
Zero-point corrected Gibbs free energy=-239.218334

C	0.13118	0.98784	0.19723
H	0.00234	1.95768	0.66587
C	1.24045	0.24339	0.52761
H	1.97246	0.68231	1.22199
O	1.53383	-0.89438	-0.02901
C	-1.82281	-0.61813	0.35666
H	-2.17181	-0.12829	1.26988
H	-1.14925	-1.43047	0.64227
H	-2.68810	-1.04118	-0.16439
Li	1.15023	0.00957	-1.49619

Electronic Energy = -239.306194978
Zero-point corrected electronic energy=-239.201585
Zero-point corrected Gibbs free energy=-239.231924

TS-B1

C	-1.06885	0.39148	-0.51844
H	-0.82768	-0.14003	-1.46317
H	-1.73915	1.19882	-0.83021
C	0.13118	0.98784	0.19723
H	0.00234	1.95768	0.66587
C	1.24045	0.24339	0.52761
H	1.97246	0.68231	1.22199
O	1.53383	-0.89438	-0.02901
C	-1.82281	-0.61813	0.35666
H	-2.17181	-0.12829	1.26988
H	-1.14925	-1.43047	0.64227
H	-2.68810	-1.04118	-0.16439
Li	1.15023	0.00957	-1.49619

One imaginary frequency: -518.46 cm^{-1}
Electronic Energy = -239.179240625
Zero-point corrected electronic energy=-239.080402
Zero-point corrected Gibbs free energy=-239.110387

TS-C1

H	1.77076	-0.74353	-1.16955
H	2.84244	0.75060	-0.87552
C	1.17527	0.51455	0.41136
H	1.36623	1.40178	1.00858
C	0.00298	-0.28922	0.78890
H	-0.37943	-0.15145	1.80765
O	-0.38445	-1.27264	0.10506
C	-1.79999	1.03494	-0.24135
H	-2.25005	2.01841	-0.23601
H	-2.17013	0.32608	0.48580
H	-0.92199	0.90183	-0.85311
Li	-1.76627	-0.94913	-1.04765

One imaginary frequency: -562.97 cm^{-1}
Electronic Energy = -239.208655099
Zero-point corrected electronic energy=-239.109595
Zero-point corrected Gibbs free energy=-239.140078

TS-D1

C	0.21820	1.18899	0.49945
H	0.39968	0.54535	1.35224
H	0.87519	2.04593	0.40687
C	-0.88182	1.03914	-0.27663
H	-1.17120	1.78613	-1.00898
C	-1.65065	-0.18399	-0.20580
H	-2.68863	-0.18063	-0.57201
O	-1.17404	-1.24899	0.21085
C	2.49981	-0.32527	-0.23735
H	2.99615	0.23710	0.56495

TS-E1

C	-0.53397	1.33960	0.27729
H	0.20894	1.11330	1.03627
H	-0.78289	2.38668	0.14944
C	-1.16275	0.35380	-0.49647
H	-1.93192	0.61705	-1.21470
C	-0.63738	-0.94673	-0.44019
H	-0.86682	-1.71320	-1.18162
O	0.33659	-1.11259	0.41257
C	1.88314	0.35448	-0.25429
H	2.48509	-0.47390	0.09808

H	3.14035	-1.19900	-0.44538
H	2.52297	0.29806	-1.14060
Li	0.73484	-1.28475	0.15937

One imaginary frequency: -168.56 cm^{-1}
Electronic Energy = -239.230416192
Zero-point corrected electronic energy=-239.132674
Zero-point corrected Gibbs free energy=-239.163993

H	1.56234	0.29563	-1.28958
H	2.22325	1.33589	0.06652
Li	-0.96165	-0.42253	1.50567

One imaginary frequency: -440.49 cm^{-1}
Electronic Energy = -239.169385182
Zero-point corrected electronic energy=-239.070403
Zero-point corrected Gibbs free energy=-239.099978

2. Energies and Cartesian coordinates of M062x/6-311++G(d,p) optimized geometries for stationary points of the 3-methoxypropene mechanism at 298.15 K

A1

C	1.59552	-0.88291	-0.02214
H	0.84160	-1.65687	0.09152
H	2.59177	-1.23128	-0.25037
C	1.21649	0.41223	-0.42229
H	1.97617	1.06223	-0.85083
C	0.01192	1.02703	-0.15232
H	-0.29145	2.01993	-0.44819
O	-0.96535	0.24687	0.51506
C	-1.74322	-0.57971	-0.34695
H	-1.09329	-1.17969	-0.98902
H	-2.38970	0.04604	-0.96721
H	-2.35371	-1.22831	0.28250
Li	0.65240	0.11107	1.55780

Electronic Energy = -239.3084429
Zero-point corrected electronic energy= -239.205094
Zero-point corrected Gibbs free energy= -239.234448

B1

C	-0.42141	1.50051	-0.00010
H	0.56811	1.04148	0.00013
H	-0.46900	2.58361	-0.00022
C	-1.54416	0.77653	-0.00014
H	-2.52355	1.24219	-0.00035
C	-1.53099	-0.69229	0.00015
H	-2.51554	-1.18718	-0.00018
O	-0.53380	-1.39120	0.00008
C	2.79694	0.10102	0.00004
H	2.78081	0.76734	0.87717
H	3.80180	-0.34385	-0.00000
H	2.78073	0.76732	-0.87710
Li	1.34825	-1.28533	0.00008

Electronic Energy = -239.2938223
Zero-point corrected electronic energy= -239.196339
Zero-point corrected Gibbs free energy= -239.229729

C1

C	-1.97791	0.14499	-0.24645
H	-1.75835	1.18044	-0.48136
H	-2.99038	-0.21064	-0.39722
C	-1.01876	-0.64709	0.21636
H	-1.24492	-1.68556	0.45674
C	0.41789	-0.22362	0.44163
H	0.62272	-0.42233	1.51209
O	0.65402	1.08818	0.14222
C	1.34131	-1.15171	-0.36545
H	1.17866	-2.20567	-0.12183
H	2.38307	-0.89983	-0.15508
H	1.15303	-1.00405	-1.43227

D1

C	1.05909	0.39595	0.51478
H	0.81025	-0.13429	1.45593
H	1.72194	1.20613	0.82757
C	-0.13676	0.97913	-0.21682
H	-0.00935	1.93804	-0.70330
C	-1.24178	0.22443	-0.52924
H	-1.97486	0.64671	-1.23012
O	-1.52631	-0.89804	0.05015
C	1.82489	-0.61502	-0.34826
H	2.17815	-0.12968	-1.25989
H	1.15748	-1.43016	-0.63326
H	2.68608	-1.03055	0.18137

Li 0.94959 2.60229 -0.26513 Electronic Energy = -239.3502262 Zero-point corrected electronic energy= -239.246675 Zero-point corrected Gibbs free energy= -239.277419	Li -1.13059 0.07040 1.47924 Electronic Energy = -239.260866 Zero-point corrected electronic energy= -239.291038 Zero-point corrected Gibbs free energy= -239.3653035
TS-B1 C -1.70609 -0.81900 0.02882 H -1.50847 -1.20350 -0.97520 H -2.56645 -1.27420 0.49744 C -1.30122 0.45509 0.38255 H -1.86951 0.98055 1.14734 C -0.15407 1.09749 -0.11360 H 0.11628 2.10136 0.20376 O 0.73381 0.40136 -0.77144 C 1.93403 -0.45990 0.54765 H 2.55113 0.42596 0.52875 H 1.27141 -0.53002 1.40810 H 2.50533 -1.36689 0.32432 Li 0.33130 -1.32875 -0.67851 One imaginary frequency: -521.09 cm^{-1} Electronic Energy = -239.2375718 Zero-point corrected electronic energy = -239.13900 Zero-point corrected Gibbs free energy= -239.168898	TS-C1 C -1.98798 -0.16400 -0.59026 H -1.80356 0.74963 -1.14429 H -2.85230 -0.75854 -0.85814 C -1.17118 -0.52299 0.40285 H -1.34059 -1.41871 0.99001 C -0.00648 0.29224 0.77674 H 0.37972 0.14998 1.79174 O 0.37251 1.27368 0.09694 C 1.81475 -1.02558 -0.24118 H 2.26157 -2.00832 -0.22775 H 2.17039 -0.32055 0.49519 H 0.94557 -0.89162 -0.86310 Li 1.78815 0.94357 -1.01603 One imaginary frequency: -562.95 cm^{-1} Electronic Energy = -239.2684903 Zero-point corrected electronic energy= -239.169971 Zero-point corrected Gibbs free energy= -239.200531
TS-D1 C 0.20500 1.19746 0.49984 H 0.39612 0.55137 1.34593 H 0.85160 2.06056 0.41215 C -0.88904 1.03739 -0.27508 H -1.18846 1.78101 -1.00381 C -1.64095 -0.19533 -0.20796 H -2.67593 -0.20193 -0.57888 O -1.15584 -1.24976 0.20729 C 2.48729 -0.31347 -0.24191 H 3.00157 0.24684 0.54817 H 3.12790 -1.18083 -0.46800 H 2.49506 0.31316 -1.14084 Li 0.75501 -1.30947 0.19254 One imaginary frequency: -173.45 cm^{-1} Electronic Energy = -239.2883993 Zero-point corrected electronic energy= -239.191167 Zero-point corrected Gibbs free energy= -	TS-E1 C -0.54672 1.33204 0.26854 H 0.17297 1.11756 1.05027 H -0.81168 2.37322 0.13991 C -1.16185 0.33548 -0.49853 H -1.93131 0.58313 -1.21887 C -0.62216 -0.95585 -0.43056 H -0.84354 -1.72916 -1.16442 O 0.35596 -1.09848 0.41700 C 1.87136 0.36767 -0.25358 H 2.49010 -0.44714 0.09593 H 1.55974 0.30924 -1.28982 H 2.18788 1.35248 0.07429 Li -0.97185 -0.41585 1.48717 One imaginary frequency: -449.51 cm^{-1} Electronic Energy = -239.2295676 Zero-point corrected electronic energy= -239.13069 Zero-point corrected Gibbs free energy= -

239.222552	239.160115

3. Energies and Cartesian coordinates of M062x/cc-pVTZ optimized geometries for stationary points of the 3-methoxypropene mechanism at 298.15 K

A1				B1			
C	1.58899	-0.88280	-0.01620	C	-0.40492	1.49738	0.00015
H	0.83561	-1.65196	0.10959	H	0.58003	1.03287	0.00041
H	2.58317	-1.23388	-0.23874	H	-0.44558	2.57876	0.00022
C	1.21356	0.40694	-0.42117	C	-1.52922	0.78305	-0.00013
H	1.97260	1.05056	-0.85493	H	-2.50309	1.25542	-0.00030
C	0.01403	1.02592	-0.15546	C	-1.53024	-0.68284	-0.00018
H	-0.28624	2.01284	-0.46636	H	-2.51893	-1.16533	-0.00019
O	-0.96854	0.25492	0.51319	O	-0.54293	-1.39400	0.00004
C	-1.73253	-0.58450	-0.34505	C	2.78382	0.09092	-0.00003
H	-1.07496	-1.18523	-0.97497	H	2.76326	0.75744	0.87417
H	-2.37737	0.02800	-0.97689	H	3.78854	-0.34833	0.00045
H	-2.34332	-1.23166	0.28247	H	2.76368	0.75647	-0.87497
Li	0.64486	0.12622	1.54719	Li	1.33298	-1.28214	0.00034
Electronic Energy = -239.3327995 Zero-point corrected electronic energy= -239.229276 Zero-point corrected Gibbs free energy= -239.258537				Electronic Energy = -239.220053 Zero-point corrected electronic energy= -239.253409 Zero-point corrected Gibbs free energy= -239.3176698			
C1				D1			
C	-1.97391	0.11398	-0.24433	C	1.06082	0.39821	0.51067
H	-1.77431	1.15202	-0.47706	H	0.82316	-0.12290	1.45727
H	-2.97841	-0.25753	-0.39566	H	1.72751	1.20644	0.81179
C	-1.00426	-0.65982	0.21499	C	-0.13841	0.98095	-0.21075
H	-1.21259	-1.70038	0.45181	H	-0.01438	1.94123	-0.68998
C	0.42332	-0.21722	0.44104	C	-1.24156	0.23069	-0.52140
H	0.63050	-0.41954	1.50842	H	-1.97749	0.65916	-1.21249
O	0.64184	1.09720	0.14801	O	-1.52214	-0.89794	0.04722
C	1.35747	-1.12906	-0.36670	C	1.81428	-0.61759	-0.35206
H	1.20690	-2.18370	-0.12839	H	2.16028	-0.13862	-1.26729
H	2.39391	-0.86627	-0.15472	H	1.14326	-1.43033	-0.62721
H	1.16949	-0.98020	-1.43134	H	2.67726	-1.03290	0.17018
Li	0.87135	2.61022	-0.27570	Li	-1.11109	0.04930	1.47374
Electronic Energy = -239.3737382 Zero-point corrected electronic energy= -239.270105 Zero-point corrected Gibbs free energy= -239.300888				Electronic Energy = -239.38977 Zero-point corrected electronic energy= -239.285157 Zero-point corrected Gibbs free energy= -239.31524			
TS-B1				TS-C1			

C	-1.71405	-0.81279	0.02522	C	-1.99309	-0.16281	-0.57866
H	-1.50807	-1.20948	-0.96956	H	-1.82081	0.75619	-1.12368
H	-2.57885	-1.25872	0.48956	H	-2.85513	-0.75841	-0.84313
C	-1.29808	0.45258	0.37947	C	-1.16356	-0.52689	0.39631
H	-1.86484	0.97856	1.14221	H	-1.32066	-1.42818	0.97438
C	-0.15018	1.09309	-0.10829	C	-0.00238	0.28924	0.76737
H	0.12162	2.09025	0.22265	H	0.38700	0.14142	1.77840
O	0.73858	0.40395	-0.77018	O	0.37028	1.27721	0.09578
C	1.93267	-0.46566	0.54208	C	1.81712	-1.02117	-0.24842
H	2.55202	0.41603	0.52878	H	2.24310	-2.01059	-0.21894
H	1.26846	-0.53322	1.39888	H	2.15427	-0.32855	0.50485
H	2.50167	-1.37350	0.32593	H	0.94098	-0.88723	-0.85645
Li	0.32572	-1.31494	-0.66929	Li	1.78681	0.94249	-1.00042
One imaginary frequency: -525.22 cm^{-1} Electronic Energy = -239.2614803 Zero-point corrected electronic energy= -239.162767 Zero-point corrected Gibbs free energy= -239.192652				One imaginary frequency: -559.16 cm^{-1} Electronic Energy = -239.2932626 Zero-point corrected electronic energy= -239.194547 Zero-point corrected Gibbs free energy= -239.225063			
TS-D1				TS-E1			
C	0.20407	1.19706	0.49544	C	-0.54212	1.32769	0.26751
H	0.39933	0.55024	1.33735	H	0.16999	1.11532	1.05293
H	0.84825	2.05925	0.40708	H	-0.80527	2.36718	0.13834
C	-0.88662	1.03391	-0.27607	C	-1.16088	0.33222	-0.49232
H	-1.18674	1.77515	-1.00391	H	-1.93140	0.57927	-1.20849
C	-1.64093	-0.19424	-0.20545	C	-0.62239	-0.95444	-0.42607
H	-2.67519	-0.19553	-0.57347	H	-0.84430	-1.72567	-1.15887
O	-1.16175	-1.24992	0.20970	O	0.36494	-1.09338	0.41262
C	2.49419	-0.31894	-0.23729	C	1.85323	0.36900	-0.25606
H	2.99434	0.23587	0.56259	H	2.48724	-0.42470	0.10780
H	3.13356	-1.18593	-0.45553	H	1.55980	0.29002	-1.29387
H	2.51797	0.31109	-1.13085	H	2.15179	1.36165	0.05686
Li	0.74607	-1.28587	0.17313	Li	-0.95815	-0.42093	1.48200
One imaginary frequency: -171.16 cm^{-1} Electronic Energy = -239.3125324 Zero-point corrected electronic energy= -239.215332 Zero-point corrected Gibbs free energy= -239.246932				One imaginary frequency: -456.29 cm^{-1} Electronic Energy = -239.2537962 Zero-point corrected electronic energy= -239.154579 Zero-point corrected Gibbs free energy= -239.183999			

4. Energies and Cartesian coordinates of M062x/6-31+G(d,p) optimized geometries for stationary points of the 5,6-dihydro-2H-pyranmechanism at 298.15 K

A2				B2			
C	-0.19042	1.38013	0.09442	C	0.56493	1.29462	-0.10483

C	1.03580	0.86555	-0.37279
H	-0.35706	2.44883	0.01672
C	-1.42577	0.47895	0.02786
C	1.33522	-0.48048	-0.22200
H	1.82075	1.53031	-0.72804
O	0.26510	-1.23505	0.32695
H	2.14025	-1.04956	-0.66455
C	-0.99218	-0.93936	-0.32808
H	-2.12334	0.82604	-0.74996
H	-2.00100	0.47327	0.96356
H	-1.70108	-1.69957	0.00856
H	-0.83169	-1.04544	-1.40642
Li	0.78549	0.18929	1.58266

Electronic Energy = -277.348069382
Zero-point corrected electronic energy=-277.235849
Zero-point corrected Gibbs free energy=-277.264849

C	-0.78315	1.22281	0.05398
H	0.91090	2.32779	-0.19307
C	1.70339	0.32623	-0.14065
C	-1.72721	0.11922	0.16064
H	-1.29866	2.17881	0.12969
O	-1.59683	-1.06241	-0.15338
H	-2.71867	0.42718	0.53779
C	1.52856	-1.12364	0.28578
H	2.49818	0.86632	0.41412
H	2.06180	0.39009	-1.18594
H	2.50328	-1.61541	0.17053
H	1.31952	-1.13787	1.36957
Li	-0.07360	-1.99103	-0.51507

Electronic Energy = -277.332094659
Zero-point corrected electronic energy=-277.223976
Zero-point corrected Gibbs free energy=-277.255451

C2

C	0.04659	0.99953	-0.73577
H	-1.76199	1.84605	0.10216
C	-1.41519	-0.39335	0.49682
C	0.80110	-0.33180	-0.56460
H	0.47993	1.86711	-1.23087
O	1.69816	-0.18599	0.47859
H	1.29883	-0.64382	-1.49820
C	-0.37554	-1.27977	-0.22225
H	-2.44683	-0.68415	0.27304
H	-1.31930	-0.43589	1.59112
H	-0.02132	-2.11652	0.38377
H	-0.82195	-1.67220	-1.14380
Li	1.08981	1.13284	1.35797

Electronic Energy = -277.385367383
Zero-point corrected electronic energy=-277.273858
Zero-point corrected Gibbs free energy=-277.303954

D2

C	0.40483	1.08494	-0.02907
H	-0.69886	-0.05884	-1.58024
C	-2.07492	0.37359	0.05428
C	1.65497	0.57905	0.16371
H	0.20670	2.13906	0.13148
O	1.99833	-0.66673	-0.01577
H	2.44480	1.26255	0.50345
C	-1.30281	-0.86768	0.40736
H	-2.93147	0.25489	-0.59957
H	-2.18789	1.11619	0.83621
H	-0.90085	-0.92557	1.41601
H	-1.69211	-1.79975	-0.00518
Li	0.63818	-1.66447	-0.34665

Electronic Energy = -277.381591143
Zero-point corrected electronic energy=-277.271066
Zero-point corrected Gibbs free energy=-277.301788

TS-B2

C	-0.25473	1.33260	0.22520
C	1.03749	1.02024	-0.23099
H	-0.55224	2.37760	0.20049
C	-1.45965	0.36719	-0.07135
C	1.48076	-0.30612	-0.21881
H	1.70187	1.79609	-0.60807
O	0.75452	-1.19115	0.40258
H	2.30646	-0.65236	-0.84497

TS-C2

C	0.90332	1.14961	-0.16420
C	-1.24293	-0.07278	0.26943
H	-0.90375	2.11738	0.39026
O	-1.93211	-0.39733	-0.68451
C	1.58672	-0.17134	-0.45311
H	1.44919	2.08413	-0.29768
C	0.77035	-1.32082	0.14755
H	1.72548	-0.23377	-1.54326

C	-1.16089	-0.99976	-0.51096
H	-1.92338	0.91079	-0.90613
H	-2.21183	0.38967	0.73609
H	-1.82390	-1.80830	-0.21799
H	-0.62356	-1.14279	-1.43766
Li	-0.25581	-0.27548	1.56635

One Imaginary frequency: -369.04cm^{-1}
Electronic Energy = -277.289014930
Zero-point corrected electronic energy=-277.181687
Zero-point corrected Gibbs free energy=-277.210996

H	2.60437	-0.12995	-0.04031
H	0.21233	-1.88855	-0.59440
Li	0.22846	-0.30279	1.80659
H	1.42970	-2.03051	0.67328
H	-1.58183	-0.40409	1.29796

One Imaginary frequency: -195.02cm^{-1}
Electronic Energy = -277.295862695
Zero-point corrected electronic energy=-277.188892
Zero-point corrected Gibbs free energy=-277.219185

TS-D2

C	-0.50925	1.07826	-0.06749
C	0.85693	1.08956	-0.27517
H	-1.05870	1.88407	-0.55597
C	-1.35358	0.17861	0.75952
C	1.75472	0.04039	0.09878
H	1.29319	1.93100	-0.80590
O	1.40629	-1.14892	0.25027
H	2.82648	0.28716	0.17910
C	-1.85929	-0.66754	-0.41961
H	-2.10235	0.73302	1.34067
H	-0.74655	-0.41980	1.44422
H	-2.10885	-1.68720	-0.09570
H	-2.71096	-0.21275	-0.92367
Li	0.00675	-1.21327	-1.05368

One Imaginary frequency: -405.22cm^{-1}
Electronic Energy = -277.327014090
Zero-point corrected electronic energy=-277.219875
Zero-point corrected Gibbs free energy=-277.250443

TS-E2

C	1.04597	1.00839	-0.02339
H	-0.57479	2.32438	0.39970
C	-1.42980	0.41736	-0.38557
C	1.47753	-0.30856	-0.23577
H	1.78325	1.76119	0.24615
O	0.53631	-1.23550	-0.38647
H	2.48445	-0.64074	0.03322
C	-1.22627	-0.89498	0.31613
H	-1.44553	0.27661	-1.47152
H	-2.39500	0.85265	-0.09873
H	-1.55447	-0.86768	1.36417
H	-1.47954	-1.83533	-0.15525
Li	0.51534	-0.42876	1.46200

One Imaginary frequency: -561.44 cm^{-1}
Electronic Energy = -277.274747689
Zero-point corrected electronic energy=-277.166302
Zero-point corrected Gibbs free energy=-277.195527

TS-E3

C	-0.43380	1.20320	0.05191
C	0.91865	1.02623	-0.34279
H	-0.83697	2.18046	-0.20497
C	-1.54068	0.15908	0.35256
C	1.55343	-0.21537	-0.25346
H	1.43789	1.86353	-0.79761
O	0.89899	-1.18230	0.30444
H	2.51752	-0.40333	-0.73520
C	-1.41314	-0.91057	-0.63387
H	-2.47193	0.72446	0.23121
H	-1.57459	-0.23783	1.37894
H	-1.15304	-1.92593	-0.37457

[1,2]-Wittig concerted transition state

C	1.07266	0.38373	-0.48444
C	-0.02829	1.27740	-0.41319
C	-1.20313	0.80442	0.15826
C	-1.25402	-0.71862	0.22776
C	-0.05474	-1.19108	-0.58296
H	0.28363	-2.20580	-0.38642
O	1.24152	-0.59377	0.58762
H	0.03714	2.26462	-0.87065
H	-2.08786	1.41228	0.29522
H	-2.18156	-1.10645	-0.21595
H	-1.18107	-1.14215	1.23786
Li	0.74112	0.86963	1.50074

H	-1.42092	-0.63466	-1.68321	H	1.97870	0.62631	-1.03249
Li	0.60111	0.10544	1.56792	H	-0.19935	-1.04262	-1.66334
One Imaginary frequency: -317.54 cm^{-1} Electronic Energy = -277.279422497 Zero-point corrected electronic energy=-277.172166 Zero-point corrected Gibbs free energy=-277.201794				One Imaginary frequency: -1268.42 cm^{-1} Electronic Energy = -277.229678059 Zero-point corrected electronic energy= -277.121255 Zero-point corrected Gibbs free energy=-277.150367			

5. Energies and Cartesian coordinates of M062x/6-311++G(d,p) optimized geometries for stationary points of the 5,6-dihydro-2H-pyranmechanism at 298.15 K

A2				B2			
C	-0.18380	1.37986	0.09330	C	0.56065	1.29655	-0.11734
C	1.03778	0.86040	-0.37022	C	-0.78307	1.22446	0.04570
H	-0.34626	2.44711	0.01511	H	0.90931	2.32522	-0.22380
C	-1.42297	0.48427	0.03105	C	1.69541	0.32751	-0.12550
C	1.33168	-0.48446	-0.22162	C	-1.71506	0.11442	0.17253
H	1.82339	1.51995	-0.72764	H	-1.30324	2.17679	0.11109
O	0.25916	-1.23514	0.32526	O	-1.58141	-1.05759	-0.15295
H	2.13206	-1.05326	-0.66867	H	-2.69663	0.41255	0.57881
C	-0.99729	-0.93438	-0.32768	C	1.51300	-1.12623	0.28323
H	-2.11827	0.83572	-0.74350	H	2.46864	0.86106	0.46229
H	-1.99476	0.48132	0.96612	H	2.09297	0.40470	-1.15346
H	-1.70785	-1.68999	0.00854	H	2.49418	-1.60766	0.20604
H	-0.83920	-1.03888	-1.40406	H	1.26220	-1.14794	1.35593
Li	0.79505	0.18166	1.57435	Li	-0.06727	-1.99475	-0.55502
Electronic Energy = -277.4137971 Zero-point corrected electronic energy= -277.301767 Zero-point corrected Gibbs free energy = -277.330738				Electronic Energy = -277.3978002 Zero-point corrected electronic energy= -277.290064 Zero-point corrected Gibbs free energy= -277.321515			
C2				D2			
C	-1.09829	0.99278	-0.03771	C	-0.70382	-0.22073	0.52153
C	0.04575	1.00006	-0.73317	C	0.40569	-1.08719	0.03527
H	-1.75925	1.84332	0.10073	H	-0.70241	0.05665	1.58056
C	-1.41422	-0.39331	0.49569	C	-2.06982	-0.37183	-0.05980
C	0.80019	-0.33108	-0.56496	C	1.64989	-0.57719	-0.16447
H	0.47645	1.86580	-1.22920	H	0.21050	-2.14085	-0.11682
O	1.69668	-0.18441	0.47626	O	1.98519	0.66731	0.00816
H	1.29563	-0.64177	-1.49683	H	2.43921	-1.25815	-0.50417
C	-0.37452	-1.28005	-0.22145	C	-1.29139	0.86581	-0.41019
H	-2.44348	-0.68219	0.26896	H	-2.92774	-0.24775	0.58727
H	-1.32158	-0.43559	1.58791	H	-2.17888	-1.11437	-0.83902
H	-0.01908	-2.11226	0.38599	H	-0.88079	0.91975	-1.41288
H	-0.81889	-1.67395	-1.14049	H	-1.68194	1.79709	-0.00275

Li 1.08773 1.12718 1.36082 Electronic Energy = -277.4501586 Zero-point corrected electronic energy= -277.338819 Zero-point corrected Gibbs free energy= -277.368824	Li 0.63242 1.66532 0.36951 Electronic Energy = -277.4464898 Zero-point corrected electronic energy= -277.336321 Zero-point corrected Gibbs free energy= -277.366994
TS-B2 C -0.25392 1.33285 0.22272 C 1.03788 1.01672 -0.22826 H -0.55176 2.37536 0.18895 C -1.45601 0.36539 -0.07203 C 1.47824 -0.30645 -0.21177 H 1.70236 1.78864 -0.60678 O 0.74574 -1.18766 0.40310 H 2.30519 -0.65337 -0.83202 C -1.14693 -0.99720 -0.51477 H -1.92759 0.90261 -0.90417 H -2.20411 0.38108 0.73715 H -1.80383 -1.81064 -0.22907 H -0.61215 -1.12836 -1.44237 Li -0.27656 -0.27397 1.56272 One imaginary frequency: -380.39 cm^{-1} Electronic Energy = -277.3547876 Zero-point corrected electronic energy = -277.247696 Zero-point corrected Gibbs free energy= -277.27698	TS-C2 C -0.39717 1.16775 0.21902 C 0.88432 1.15536 -0.16126 C -1.26202 -0.08034 0.26973 H -0.93006 2.10203 0.37864 O -1.94962 -0.41627 -0.66986 C 1.60387 -0.14671 -0.44069 H 1.41291 2.09883 -0.28771 C 0.81279 -1.32323 0.14040 H 1.77172 -0.19567 -1.52575 H 2.60845 -0.07782 -0.00515 H 0.25176 -1.86810 -0.61424 Li 0.23746 -0.29896 1.77445 H 1.48864 -2.03922 0.62722 H -1.56962 -0.42992 1.29932 One imaginary frequency: -169.89 cm^{-1} Electronic Energy = -277.3628838 Zero-point corrected electronic energy= -277.256219 Zero-point corrected Gibbs free energy= -277.286525
TS-D2 C -0.50181 1.08039 -0.05851 C 0.85758 1.08213 -0.27798 H -1.04954 1.89261 -0.53427 C -1.34577 0.17332 0.75938 C 1.75331 0.03057 0.10268 H 1.29719 1.91993 -0.80819 O 1.40545 -1.15170 0.24258 H 2.82156 0.28135 0.19988 C -1.86827 -0.66691 -0.42022 H -2.08778 0.72590 1.34610 H -0.74020 -0.43153 1.43619 H -2.11793 -1.68235 -0.09234 H -2.72697 -0.20513 -0.90152 Li -0.00339 -1.16140 -1.07287 One imaginary frequency: -389.45 cm^{-1} Electronic Energy = -277.3925119 Zero-point corrected electronic energy= -	TS-E2 C -0.31103 1.32274 0.05794 C 1.04414 1.00598 -0.02748 H -0.57654 2.31904 0.39192 C -1.43128 0.41377 -0.38749 C 1.47790 -0.30873 -0.22848 H 1.77869 1.76158 0.23318 O 0.54406 -1.23763 -0.37861 H 2.48726 -0.63307 0.03167 C -1.22689 -0.89595 0.31431 H -1.45030 0.27420 -1.47125 H -2.39365 0.84773 -0.09709 H -1.54301 -0.87027 1.36356 H -1.47314 -1.83653 -0.15551 Li 0.50040 -0.39614 1.45322 One imaginary frequency: -559.95 cm^{-1} Electronic Energy = -277.3413351 Zero-point corrected electronic energy= -

277.285733 Zero-point corrected Gibbs free energy= -277.316302	277.233077 Zero-point corrected Gibbs free energy= -277.262218
TS-E3 C -0.42798 1.20308 0.04411 C 0.92187 1.01745 -0.34701 H -0.82787 2.17865 -0.21593 C -1.53518 0.16488 0.35724 C 1.54687 -0.22638 -0.25089 H 1.44622 1.84719 -0.80532 O 0.88523 -1.18346 0.30496 H 2.50975 -0.41920 -0.72928 C -1.41442 -0.90533 -0.62725 H -2.46548 0.72934 0.24083 H -1.55909 -0.22867 1.38202 H -1.17389 -1.92314 -0.36707 H -1.42734 -0.63233 -1.67536 Li 0.62297 0.13122 1.55775 One imaginary frequency: -321.89 cm^{-1} Electronic Energy = -277.3459369 Zero-point corrected electronic energy= -277.239027 Zero-point corrected Gibbs free energy= -277.268602	

7. Energies and Cartesian coordinates of M062x/cc-pVTZ optimized geometries for stationary points of the 5,6-dihydro-2H-pyranmechanism at 298.15 K

A2 C -0.18539 1.37772 0.09130 C 1.03473 0.86039 -0.36654 H -0.34854 2.44247 0.01145 C -1.42012 0.48164 0.03311 C 1.33075 -0.48043 -0.21806 H 1.81863 1.51986 -0.72151 O 0.26029 -1.23639 0.32281 H 2.13320 -1.04302 -0.66428 C -0.99316 -0.93219 -0.32880 H -2.12027 0.83102 -0.73491 H -1.98716 0.47325 0.96864 H -1.70535 -1.68635 0.00118 H -0.83594 -1.03137 -1.40411 Li 0.78742 0.18083 1.56500 Electronic Energy = -277.4414481 Zero-point corrected electronic energy= -277.329313	B2 C 0.56651 1.29062 -0.12233 C -0.77413 1.22437 0.03719 H 0.92028 2.31420 -0.23691 C 1.69490 0.32067 -0.11088 C -1.70758 0.12158 0.17605 H -1.29049 2.17700 0.09276 O -1.58318 -1.05225 -0.14398 H -2.68253 0.42621 0.58837 C 1.50076 -1.13331 0.27285 H 2.44836 0.84752 0.50576 H 2.12583 0.41310 -1.12153 H 2.47874 -1.61777 0.21612 H 1.21926 -1.16847 1.33518 Li -0.07890 -1.97246 -0.58173 Electronic Energy = -277.4246008 Zero-point corrected electronic energy= -277.316773

Zero-point corrected Gibbs free energy = -277.358276	Zero-point corrected Gibbs free energy= -277.348143
C2 C -1.09596 0.99069 -0.03934 C 0.04550 0.99808 -0.73102 H -1.75335 1.84071 0.10264 C -1.41136 -0.39234 0.49367 C 0.79907 -0.32956 -0.56386 H 0.47922 1.86353 -1.22032 O 1.69490 -0.18103 0.47531 H 1.29160 -0.63980 -1.49532 C -0.37377 -1.27798 -0.22170 H -2.43892 -0.68210 0.27130 H -1.31668 -0.43304 1.58376 H -0.01968 -2.10901 0.38438 H -0.81716 -1.67134 -1.13864 Li 1.07831 1.11532 1.36107 Electronic Energy = -277.47714 Zero-point corrected electronic energy= -277.365659 Zero-point corrected Gibbs free energy= -277.395616	D2 C -0.70337 -0.21909 0.51879 C 0.40436 -1.08379 0.03585 H -0.69993 0.06205 1.57454 C -2.06764 -0.36908 -0.05850 C 1.64492 -0.57684 -0.16363 H 0.20960 -2.13528 -0.11613 O 1.98431 0.66659 0.00702 H 2.43076 -1.25974 -0.50267 C -1.28921 0.86338 -0.41049 H -2.92320 -0.24319 0.58751 H -2.17890 -1.11152 -0.83434 H -0.87716 0.91683 -1.41006 H -1.67339 1.79501 -0.00427 Li 0.63446 1.65189 0.37236 Electronic Energy = -277.4742645 Zero-point corrected electronic energy= -277.36386 Zero-point corrected Gibbs free energy= -277.394502
TS-B2 C -0.25574 1.33161 0.22123 C 1.03442 1.01657 -0.22303 H -0.55648 2.37056 0.18415 C -1.45234 0.36212 -0.06920 C 1.47576 -0.30158 -0.20770 H 1.69698 1.78765 -0.60069 O 0.74491 -1.18757 0.40116 H 2.30094 -0.64360 -0.83009 C -1.13904 -0.99384 -0.51624 H -1.93244 0.90099 -0.89239 H -2.19296 0.36954 0.74431 H -1.79727 -1.80648 -0.23939 H -0.60303 -1.11833 -1.44129 Li -0.28447 -0.28303 1.54527 One imaginary frequency: -386.35 cm^{-1} Electronic Energy = -277.3815955 Zero-point corrected electronic energy= -277.274297 Zero-point corrected Gibbs free energy= -277.303534	TS-C2 C -0.39327 1.16382 0.21129 C 0.88589 1.15039 -0.16198 C -1.25971 -0.07887 0.27050 H -0.92411 2.09758 0.36633 O -1.95779 -0.41184 -0.66050 C 1.60737 -0.14881 -0.43206 H 1.41378 2.09163 -0.28914 C 0.80824 -1.32300 0.13318 H 1.79719 -0.19402 -1.51164 H 2.60215 -0.08193 0.02069 H 0.24656 -1.85530 -0.62647 Li 0.23933 -0.29087 1.76005 H 1.47542 -2.04571 0.61638 H -1.55768 -0.42613 1.30213 One imaginary frequency: -159.93 cm^{-1} Electronic Energy = -277.3890688 Zero-point corrected electronic energy= -277.282248 Zero-point corrected Gibbs free energy= -277.312494
TS-D2 C -0.49991 1.07957 -0.04821	TS-E2 C -0.31377 1.31793 0.05923

C	0.85330	1.08027	-0.27528
H	-1.04686	1.89628	-0.51223
C	-1.34365	0.16577	0.75600
C	1.75171	0.03103	0.09533
H	1.28959	1.91933	-0.80177
O	1.40961	-1.15081	0.24265
H	2.81864	0.28420	0.18078
C	-1.87007	-0.66530	-0.42697
H	-2.08242	0.71296	1.34833
H	-0.74050	-0.44601	1.42529
H	-2.14509	-1.67055	-0.09681
H	-2.71605	-0.18675	-0.90991
Li	-0.00085	-1.15030	-1.06003

One imaginary frequency: -379.12 cm^{-1}
Electronic Energy = -277.4201631
Zero-point corrected electronic energy= -277.313187
Zero-point corrected Gibbs free energy= -277.343662

C	1.03845	1.00694	-0.02368
H	-0.58207	2.30857	0.40077
C	-1.42935	0.41004	-0.38855
C	1.47616	-0.30124	-0.23135
H	1.76859	1.76214	0.24096
O	0.54710	-1.23362	-0.37911
H	2.48424	-0.61934	0.03478
C	-1.22321	-0.89354	0.31542
H	-1.44594	0.26794	-1.46988
H	-2.39129	0.84265	-0.10339
H	-1.54468	-0.86324	1.36039
H	-1.46605	-1.83507	-0.14880
Li	0.50360	-0.41184	1.44389

One imaginary frequency: -558.47 cm^{-1}
Electronic Energy = -277.36914134
Zero-point corrected electronic energy= -277.260708
Zero-point corrected Gibbs free energy= -277.289843

TS-E3

C	-0.42899	1.20076	0.04158
C	0.92087	1.01845	-0.33692
H	-0.82969	2.17228	-0.22286
C	-1.53248	0.16455	0.35497
C	1.54468	-0.22140	-0.24521
H	1.44466	1.84829	-0.79032
O	0.88024	-1.18389	0.29813
H	2.50673	-0.41041	-0.72237
C	-1.40114	-0.90200	-0.62652
H	-2.46266	0.72476	0.23714
H	-1.55881	-0.22647	1.37864
H	-1.18074	-1.92172	-0.36717
H	-1.41372	-0.62997	-1.67225
Li	0.61155	0.11743	1.54892

One imaginary frequency: -333.32 cm^{-1}
Electronic Energy = -277.3731706
Zero-point corrected electronic energy= -277.266059
Zero-point corrected Gibbs free energy= -277.295603

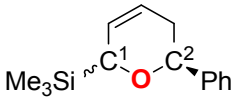
[1,2]-Wittig concerted transition state

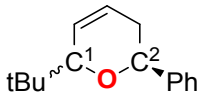
C	1.07710	0.36417	-0.48061
C	-0.00704	1.26917	-0.41143
C	-1.18284	0.82435	0.16367
C	-1.26561	-0.69330	0.23307
C	-0.08758	-1.18662	-0.58455
H	0.23567	-2.20201	-0.39461
O	1.23431	-0.61783	0.58567
H	0.07595	2.25017	-0.86994
H	-2.05055	1.44863	0.30110
H	-2.19860	-1.06221	-0.20564
H	-1.19714	-1.11854	1.23803
Li	0.76915	0.86322	1.47127
H	1.97973	0.59524	-1.03149
H	-0.23127	-1.02493	-1.65753

One imaginary frequency: - 1260.72 cm^{-1}
Electronic Energy = -277.3232615
Zero-point corrected electronic energy= -277.214844
Zero-point corrected Gibbs free energy= -277.243882

8. Energies and Cartesian coordinates of optimized geometries for stationary points of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism obtained at 195 K in the gas phase at M062X/6-31+G(d,p) level of theory

Numbering system followed for the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism





Reactants

Silicon analogues				Carbon Analogues			
1a				1aC			
C	-2.68663	-2.12425	-0.87777	C	-2.38211	-2.00771	-0.64047
Si	-2.63391	-0.55403	0.15251	C	-3.51594	0.22179	-0.45330
C	-3.58376	0.83550	-0.68046	C	-2.95796	-1.09638	1.60933
C	-3.29536	-0.87398	1.88798	C	-1.10682	-0.05974	0.25760
C	-0.80258	-0.01418	0.28990	H	-0.42296	-0.78151	0.74425
H	-0.22761	-0.81972	0.78560	C	-1.06970	1.22583	1.04244
C	-0.64948	1.25211	1.07543	C	-0.47560	2.32787	0.58237
C	-0.05324	2.33913	0.57851	C	0.21652	2.34913	-0.75422
C	0.58183	2.31681	-0.78744	C	0.50547	0.92204	-1.21454
C	0.83776	0.87460	-1.21979	H	0.70488	0.92096	-2.29188
H	1.02904	0.84610	-2.29831	C	1.67517	0.22708	-0.52601
C	1.99109	0.16496	-0.52072	C	1.95377	-1.09154	-0.90621
C	2.20475	-1.18181	-0.83850	C	2.99912	-1.79799	-0.32067
C	3.23806	-1.90090	-0.24652	C	3.78508	-1.19314	0.66159
C	4.07753	-1.28007	0.67948	C	3.51214	0.11446	1.05119
C	3.87031	0.05679	1.00639	C	2.46031	0.81938	0.46235
C	2.83009	0.77380	0.41227	O	-0.68023	0.14243	-1.08416
O	-0.36861	0.12478	-1.06413	H	-3.34441	-2.53038	-0.66482
H	-3.71546	-2.46402	-1.03466	H	-1.63738	-2.68654	-0.20774
H	-2.13330	-2.93275	-0.38888	H	-2.08238	-1.78123	-1.66620
H	-2.22965	-1.94333	-1.85513	H	-4.49561	-0.26398	-0.52033
H	-4.63141	0.56268	-0.84269	H	-3.19526	0.49812	-1.46155
H	-3.13287	1.06203	-1.65162	H	-3.63034	1.13989	0.13306
H	-3.55683	1.74665	-0.07440	H	-3.87666	-1.68981	1.55656
H	-4.31859	-1.26103	1.84097	H	-3.17588	-0.21417	2.21870
H	-3.31642	0.04269	2.48609	H	-2.20123	-1.69654	2.12819
H	-2.68505	-1.61251	2.41823	H	-1.52586	1.22185	2.02892
H	-1.05603	1.25634	2.08543	H	-0.47836	3.23771	1.17841
H	0.00241	3.25203	1.16646	H	1.13812	2.93978	-0.71306
H	1.51226	2.89505	-0.79829	H	-0.42677	2.83108	-1.50057
H	-0.08180	2.78392	-1.52538	H	1.32833	-1.56135	-1.66197
H	1.53967	-1.66203	-1.55239	H	3.20240	-2.81926	-0.62853
H	3.39040	-2.94417	-0.50620	H	4.60260	-1.74005	1.12115
H	4.88590	-1.83634	1.14402	H	4.11308	0.59003	1.82036
H	4.51440	0.54554	1.73115	H	2.25190	1.83203	0.79339
H	2.67231	1.80990	0.69530	C	-2.50053	-0.72543	0.19305
Electronic Energy = -909.978426312 Zero-point corrected electronic energy=-909.672755 Zero-point corrected Gibbs free energy=-909.698797				Electronic Energy = -658.5900815 Zero-point corrected electronic energy=-658.272311 Zero-point corrected Gibbs free energy=-658.296355			
1b				1bC			

C	4.39389	-0.29925	-0.04388
Si	2.57998	-0.77532	0.14923
C	2.11553	-0.74943	1.97495
C	2.25004	-2.47325	-0.58236
C	1.55444	0.48564	-0.88143
H	1.90230	0.34886	-1.91751
C	1.77711	1.91645	-0.50107
C	0.79104	2.71513	-0.08455
C	-0.61722	2.20099	0.04932
C	-0.59893	0.67171	0.14408
H	-0.13966	0.39809	1.10735
C	-1.98856	0.08560	0.08181
C	-2.79374	0.09753	1.22399
C	-4.09826	-0.38794	1.17715
C	-4.61007	-0.89583	-0.01646
C	-3.80916	-0.91407	-1.15701
C	-2.50433	-0.42536	-1.11044
O	0.16876	0.13081	-0.91875
H	5.04169	-1.06287	0.39917
H	4.67186	-0.19982	-1.09869
H	4.61077	0.65062	0.45542
H	2.85749	-1.31062	2.55361
H	2.08660	0.27299	2.36614
H	1.13996	-1.21443	2.14802
H	2.76601	-3.25788	-0.01980
H	1.17677	-2.68703	-0.56569
H	2.58706	-2.52510	-1.62272
H	2.79668	2.28873	-0.58184
H	0.99598	3.75250	0.16761
H	-1.10122	2.61591	0.94131
H	-1.22905	2.49792	-0.81279
H	-2.39381	0.48519	2.15896
H	-4.71188	-0.37655	2.07280
H	-5.62523	-1.27845	-0.05548
H	-4.20075	-1.31295	-2.08801
H	-1.87200	-0.44448	-1.99167

Electronic Energy = -909.977578062
Zero-point corrected electronic energy=-909.671443
Zero-point corrected Gibbs free energy=-909.697365

C	-2.69666	0.40867	1.12892
C	-4.01796	-0.02627	1.06160
C	-4.44841	-0.78101	-0.02911
C	-3.54975	-1.09581	-1.04648
C	-2.22791	-0.65691	-0.98030
C	-1.79337	0.10067	0.10845
H	-2.36138	0.98906	1.98627
H	-4.70874	0.21734	1.86313
H	-5.47656	-1.12544	-0.08196
H	-3.87678	-1.68849	-1.89559
H	-1.51929	-0.90572	-1.76314
C	-0.38389	0.63926	0.17926
H	-0.03732	0.58634	1.22166
O	0.44117	-0.16659	-0.64872
C	1.83102	0.14584	-0.68810
C	2.40466	-2.24856	-0.28846
H	2.77958	-2.37499	-1.31106
H	2.92461	-2.96912	0.35221
H	1.33696	-2.48321	-0.28252
C	2.23025	-0.71733	1.67982
H	1.20756	-1.08065	1.82170
H	2.89000	-1.33551	2.29861
H	2.29285	0.31430	2.04474
C	4.14376	-0.49422	0.08025
H	4.40520	0.43977	0.58727
H	4.73738	-1.29389	0.53549
H	4.44608	-0.41324	-0.97118
C	2.10317	1.61138	-0.47724
H	3.14245	1.92467	-0.52241
C	-0.30727	2.10148	-0.26209
H	-0.79649	2.21154	-1.23924
H	-0.86276	2.72691	0.44572
C	1.13485	2.51640	-0.33104
H	1.38198	3.57228	-0.25176
C	2.65000	-0.81949	0.21041
H	2.13032	-0.08380	-1.72352

Electronic Energy = -658.5888944
Zero-point corrected electronic energy=-658.270896
Zero-point corrected Gibbs free energy=-658.294661

2a			
C	3.53510	-0.99415	-0.80320
C	0.61171	-1.58012	-1.43634
C	1.69979	-1.99537	1.45035
C	1.52897	0.90256	0.39139
H	2.50220	1.14816	0.84837
C	1.35134	1.80238	-0.78962

2aC			
C	3.22377	-1.31451	-0.83141
C	0.75325	-1.50160	-1.11915
C	1.79953	-1.98808	1.10284
C	1.79296	0.39081	0.30470
H	2.76460	0.58994	0.78636
C	1.66662	1.36226	-0.83521
C	0.86364	2.42440	-0.80074

C	0.36375	2.69500	-0.88484
C	-0.63472	2.85317	0.23004
C	-0.71044	1.57372	1.06389
H	-1.18707	1.80627	2.02291
C	-1.51887	0.44313	0.43694
C	-1.76359	-0.68758	1.22508
C	-2.53384	-1.74282	0.74598
C	-3.08164	-1.67815	-0.53658
C	-2.84308	-0.55934	-1.33002
C	-2.06302	0.49241	-0.84728
O	0.59102	1.14364	1.44666
H	3.81179	-2.02106	-1.06499
H	4.26761	-0.62665	-0.07687
H	3.62790	-0.39009	-1.71240
H	1.03134	-2.48566	-1.88874
H	0.47808	-0.83587	-2.22890
H	-0.37515	-1.82492	-1.03508
H	2.00038	-3.02617	1.23517
H	0.68669	-2.01341	1.86042
H	2.36930	-1.59656	2.21923
H	2.07832	1.69444	-1.59326
H	0.27842	3.32893	-1.76398
H	-1.62701	3.11404	-0.15319
H	-0.33024	3.67553	0.88869
H	-1.34419	-0.72644	2.22801
H	-2.71614	-2.61032	1.37336
H	-3.68918	-2.49560	-0.91243
H	-3.25892	-0.50379	-2.33146
H	-1.87350	1.34949	-1.48650
Si	1.77803	-0.94704	-0.10688

Electronic Energy = -909.975297847
Zero-point corrected electronic energy=-909.668926
Zero-point corrected Gibbs free energy=-909.712988

C	-0.01793	2.68403	0.38781
C	-0.33154	1.37724	1.11197
H	-0.67966	1.61322	2.12389
C	-1.40843	0.51684	0.46660
C	-1.87459	-0.57426	1.20835
C	-2.81639	-1.45065	0.67981
C	-3.31548	-1.23988	-0.60669
C	-2.87255	-0.14644	-1.34604
C	-1.92436	0.72806	-0.81169
O	0.85235	0.61842	1.35524
H	3.35068	-2.37443	-1.07464
H	4.05429	-1.01882	-0.18033
H	3.30693	-0.75417	-1.76842
H	0.93938	-2.51813	-1.48446
H	0.71710	-0.83349	-1.98696
H	-0.23016	-1.49420	-0.64382
H	1.94869	-3.03646	0.82193
H	0.82916	-1.89209	1.59580
H	2.57546	-1.71294	1.82684
H	2.30389	1.18571	-1.69760
H	0.84049	3.12095	-1.63552
H	-0.94830	3.18169	0.09506
H	0.49084	3.35849	1.08778
H	-1.46916	-0.74196	2.20372
H	-3.15949	-2.29744	1.26647
H	-4.04749	-1.92267	-1.02674
H	-3.25862	0.02473	-2.34637
H	-1.57248	1.56119	-1.41304
C	1.86566	-1.09931	-0.14314

Electronic Energy = -658.258604
Zero-point corrected electronic energy=-658.265247
Zero-point corrected Gibbs free energy=-658.5833797

2b			
C	-2.34990	-2.34725	-0.85594
Si	-2.73062	-0.69461	-0.05028
C	-2.49255	-0.77863	1.81013
C	-4.47428	-0.12646	-0.48280
C	-1.47549	0.58666	-0.72852
H	-1.58471	0.65867	-1.82732
C	-1.67751	1.93952	-0.11811
C	-0.72700	2.56223	0.58343
C	0.65417	1.97583	0.70064
C	0.87115	0.94888	-0.41490
H	0.88929	1.47692	-1.38317
C	2.16190	0.18865	-0.23539
C	3.35712	0.72177	-0.72263

2bC			
C	-4.16547	-0.41656	-0.57932
C	-2.34158	-2.11216	-0.71347
C	-2.73970	-0.88195	1.43493
C	-1.75611	0.31128	-0.56251
H	-1.82287	0.35876	-1.66725
C	-2.03259	1.68488	-0.00343
C	-1.08454	2.42812	0.56918
C	0.34470	1.96257	0.63737
C	0.55702	0.83539	-0.37726
H	0.48473	1.25970	-1.39357
C	1.90264	0.17140	-0.21327
C	3.04182	0.78202	-0.74280
C	4.30072	0.21550	-0.55697
C	4.43074	-0.97344	0.15961

C	4.56602	0.06216	-0.51045
C	4.58866	-1.14335	0.18905
C	3.39771	-1.68245	0.67330
C	2.18970	-1.01968	0.46424
O	-0.20395	0.02142	-0.41412
H	-2.98033	-3.14254	-0.44531
H	-2.51593	-2.30753	-1.93724
H	-1.30238	-2.61360	-0.68531
H	-3.16071	-1.51713	2.26455
H	-1.46031	-1.05939	2.04263
H	-2.68894	0.19341	2.27359
H	-5.20750	-0.88071	-0.17832
H	-4.73154	0.80817	0.02572
H	-4.58793	0.02972	-1.56076
H	-2.65634	2.39628	-0.25463
H	-0.92842	3.52304	1.05034
H	1.41594	2.76099	0.62811
H	0.79814	1.48058	1.67047
H	3.34043	1.65701	-1.27831
H	5.48808	0.48489	-0.89772
H	5.52888	-1.66102	0.35186
H	3.40883	-2.62335	1.21524
H	1.25744	-1.43836	0.83032

Electronic Energy = -909.980493447
Zero-point corrected electronic energy=-909.674957
Zero-point corrected Gibbs free energy=-909.701282

C	3.29657	-1.58841	0.68644
C	2.03705	-1.01900	0.50288
O	-0.45741	-0.13704	-0.20936
H	-4.85075	-1.24058	-0.35527
H	-4.56075	0.47836	-0.08948
H	-4.18340	-0.25328	-1.66338
H	-3.05620	-2.89244	-0.43044
H	-2.32570	-2.04742	-1.80786
H	-1.34604	-2.41206	-0.37806
H	-3.40889	-1.68559	1.76090
H	-1.73052	-1.10370	1.79415
H	-3.07198	0.04961	1.90502
H	-3.04697	2.06434	-0.09182
H	-1.33116	3.40463	0.97980
H	1.03224	2.78952	0.42438
H	0.59262	1.59224	1.64117
H	2.94212	1.70499	-1.31065
H	5.17799	0.69729	-0.97782
H	5.40994	-1.42021	0.30127
H	3.39083	-2.51796	1.23985
H	1.14801	-1.49654	0.90227
C	-2.75529	-0.77187	-0.09276

Electronic Energy = -658.5921303
Zero-point corrected electronic energy=-658.275027
Zero-point corrected Gibbs free energy=-658.299245

A Intermediates (Lithiated)

Silicon analogues for deprotonated C^1

1aA-C^1Li

C	-3.22917	-0.52688	1.81781
Si	-2.51095	-0.47869	0.07226
C	-1.01582	0.61515	0.07882
O	-0.39821	0.74690	-1.19678
C	0.93846	1.22910	-1.17447
H	1.19656	1.38615	-2.22847
C	1.86538	0.15127	-0.60846
C	1.45059	-1.18933	-0.63357
C	2.25273	-2.20035	-0.09581
C	3.48077	-1.88523	0.48280
C	3.90322	-0.55562	0.52269
C	3.09598	0.45460	-0.00467
C	1.01530	2.55772	-0.39808
C	0.47885	2.34425	1.00028
C	-0.65489	1.51948	1.07366
C	-2.08009	-2.24259	-0.46022
C	-3.81902	0.16135	-1.12681
H	-3.53996	0.46834	2.15194

Carbon Analogues for deprotonated C^1

1aCA-C^1Li

C	-2.18342	-1.98821	-0.45448
C	-3.57163	0.02068	-0.98993
C	-3.30275	-0.72480	1.37992
C	-1.38136	0.32083	0.13748
C	-1.05204	1.15998	1.16743
C	0.07418	2.06048	1.13183
C	0.43750	2.40751	-0.29930
C	0.52104	1.10095	-1.10887
H	0.70984	1.30715	-2.16939
C	1.62464	0.18063	-0.58982
C	1.37153	-1.18033	-0.37107
C	2.36485	-2.01915	0.15417
C	3.62728	-1.51273	0.44562
C	3.89745	-0.16131	0.21065
C	2.90250	0.67684	-0.28440
O	-0.72876	0.41951	-1.09828
H	-3.07221	-2.61466	-0.59048
H	-1.53172	-2.48073	0.27758

H	-2.51111	-0.92311	2.54386	H	-1.65964	-1.93028	-1.41349
H	-4.11280	-1.17359	1.83864	H	-4.45257	-0.62213	-1.10237
H	0.49075	-1.42328	-1.08145	H	-3.09236	0.12946	-1.96635
H	1.91171	-3.23060	-0.12981	H	-3.90251	1.00975	-0.65759
H	4.10577	-2.66814	0.90097	H	-4.15113	-1.40891	1.27538
H	4.85727	-0.30009	0.97303	H	-3.68913	0.23666	1.73171
H	3.42940	1.48527	0.05511	H	-2.63339	-1.13159	2.14659
H	0.41813	3.28328	-0.96918	H	-1.63049	1.06313	2.08446
H	2.04243	2.93844	-0.40329	H	0.05060	2.87996	1.84482
H	0.64774	3.09998	1.75930	H	1.38704	2.94749	-0.37564
H	-1.21092	1.45362	2.01141	H	-0.31995	3.03193	-0.80210
H	-1.34303	-2.69620	0.21212	H	0.39600	-1.57692	-0.62723
H	-1.67382	-2.25805	-1.47773	H	2.14616	-3.07002	0.31866
H	-2.97572	-2.87392	-0.45606	H	4.39902	-2.16314	0.84503
H	-4.68015	-0.51369	-1.18146	H	4.88089	0.24310	0.42879
H	-4.17398	1.14980	-0.81889	H	3.11917	1.72958	-0.43499
H	-3.39550	0.25707	-2.13178	C	-2.59008	-0.58705	0.03222
Li	0.92081	0.22254	1.38345	Li	0.81279	0.17938	1.53472
Electronic Energy = -916.9090183				Electronic Energy = -665.510640026			
Zero-point corrected electronic energy=-916.613593				Zero-point corrected electronic energy=-665.204061			
Zero-point corrected Gibbs free energy=-916.639166				Zero-point corrected Gibbs free energy=-665.227761			
1bA-C[1]Li				1bCA-C[1]Li			
C	4.42039	-0.03526	0.38774	C	-2.97424	0.84703	0.48788
Si	2.69365	-0.75059	0.14154	C	-4.23307	0.26066	0.37684
C	2.14350	-1.68207	1.68941	C	-4.35820	-1.04818	-0.08627
C	2.69840	-1.98927	-1.28467	C	-3.21493	-1.76509	-0.43296
C	1.54018	0.63635	-0.24217	C	-1.95504	-1.18007	-0.31617
C	1.63793	2.02700	-0.10421	C	-1.82138	0.13288	0.14542
C	0.53131	2.86183	-0.28208	H	-2.88962	1.86913	0.84608
C	-0.86447	2.33681	0.03743	H	-5.11717	0.82908	0.64911
C	-0.79255	0.83466	0.32702	H	-5.33905	-1.50429	-0.17818
H	-0.41156	0.68064	1.34715	H	-3.30226	-2.78427	-0.79751
C	-2.09916	0.09248	0.15763	H	-1.06421	-1.73612	-0.58930
C	-3.30376	0.67793	0.56169	C	-0.45476	0.75401	0.32012
C	-4.50626	-0.01514	0.44219	H	-0.09367	0.55699	1.33966
C	-4.52286	-1.30326	-0.09017	O	0.47045	0.07403	-0.56811
C	-3.32778	-1.89223	-0.49647	C	1.83637	0.32710	-0.24560
C	-2.12350	-1.20087	-0.37115	C	2.55928	-1.94972	-0.95430
O	0.18498	0.24554	-0.55854	H	3.05852	-1.58312	-1.85870
H	5.14727	-0.83564	0.56076	H	3.05368	-2.87673	-0.64162
H	4.74533	0.52760	-0.49364	H	1.51959	-2.18423	-1.20429
H	4.45043	0.63665	1.25142	C	2.01134	-1.49690	1.44244
H	2.77135	-2.56032	1.87631	H	0.95762	-1.75313	1.28337
H	2.18566	-1.03565	2.57177	H	2.54184	-2.41164	1.73201
H	1.10970	-2.02828	1.57686	H	2.07277	-0.78448	2.27195
H	3.27899	-2.88482	-1.03852	C	4.07988	-0.51391	0.42121
H	1.67440	-2.30750	-1.51074	H	4.16674	0.18374	1.26056

H	3.12298	-1.54738	-2.19237
H	2.63111	2.45655	0.02394
H	0.67829	3.93490	-0.22524
H	-1.26269	2.84370	0.92912
H	-1.59545	2.51967	-0.76345
H	-3.30581	1.68336	0.97361
H	-5.43161	0.45402	0.76272
H	-5.46029	-1.84214	-0.18676
H	-3.33024	-2.89553	-0.91205
H	-1.19220	-1.65807	-0.68777
Li	0.80509	1.43619	-1.92318

Electronic Energy = -916.9129754
Zero-point corrected electronic energy=-916.617387
Zero-point corrected Gibbs free energy=-916.64364

H	4.66100	-1.40962	0.66451
H	4.52805	-0.04757	-0.46346
C	2.08311	1.68077	-0.07219
H	3.10654	2.00394	0.10608
C	-0.37506	2.25606	0.04228
H	-1.09707	2.52102	-0.74350
H	-0.70618	2.78685	0.94840
C	1.06408	2.63261	-0.30851
H	1.32585	3.68117	-0.22016
C	2.62007	-0.89372	0.16198
Li	1.21624	1.26332	-1.91771

Electronic Energy = -665.512801981
Zero-point corrected electronic energy=-665.205986
Zero-point corrected Gibbs free energy=-665.229912

2aA-C[1]Li

C	3.22312	-1.07717	-1.37212
C	0.64403	-2.35323	-0.30763
C	2.72736	-1.32931	1.67593
C	1.21795	0.70355	-0.00044
C	1.10527	1.65000	-1.02466
C	0.36120	2.82274	-0.86291
C	-0.82289	2.84669	0.10144
C	-0.86510	1.56365	0.94157
H	-1.24117	1.77861	1.94648
C	-1.68235	0.42554	0.37569
C	-2.28299	-0.47611	1.25942
C	-3.01661	-1.56166	0.78630
C	-3.15365	-1.76106	-0.58653
C	-2.55857	-0.86814	-1.47603
C	-1.82666	0.21759	-0.99917
O	0.50903	1.12849	1.18187
H	3.70213	-2.06196	-1.39101
H	4.00483	-0.32464	-1.22602
H	2.77134	-0.91290	-2.35610
H	1.08822	-3.35077	-0.21217
H	0.21655	-2.25919	-1.31121
H	-0.18269	-2.27532	0.40715
H	3.08817	-2.36041	1.75333
H	1.99967	-1.16569	2.47783
H	3.57601	-0.65828	1.84747
H	1.70136	1.49992	-1.92466
H	0.35113	3.54764	-1.67005
H	-1.77135	2.93687	-0.44813
H	-0.79392	3.71317	0.77491
H	-2.17258	-0.32271	2.33070
H	-3.47921	-2.25006	1.48704

2aCA-C[1]Li

C	2.37952	-1.71234	-1.37191
C	0.48686	-2.14486	0.20646
C	2.75114	-1.60381	1.10068
C	1.43909	0.17014	-0.05298
C	1.52289	1.11756	-1.05200
C	1.13927	2.46411	-0.80910
C	-0.00529	2.73841	0.17084
C	-0.33769	1.47628	0.97515
H	-0.61331	1.73055	2.00260
C	-1.42501	0.59938	0.40138
C	-2.18330	-0.18905	1.27084
C	-3.15393	-1.06119	0.78486
C	-3.37999	-1.15125	-0.58814
C	-2.63772	-0.36039	-1.46379
C	-1.66480	0.50928	-0.97308
O	0.89868	0.69737	1.15293
H	2.65636	-2.77145	-1.34442
H	3.28518	-1.13233	-1.58305
H	1.67512	-1.56656	-2.19762
H	0.73755	-3.21246	0.20603
H	-0.26491	-1.95984	-0.56776
H	0.04123	-1.89921	1.17466
H	2.94087	-2.68043	1.18368
H	2.35389	-1.25410	2.05914
H	3.71067	-1.10534	0.91379
H	1.99729	0.84793	-1.99259
H	1.24358	3.16492	-1.63062
H	-0.91894	3.06048	-0.35125
H	0.23121	3.55193	0.86839
H	-1.99976	-0.12454	2.34125
H	-3.73318	-1.66813	1.47402

H	-3.72255	-2.60684	-0.96055
H	-2.66110	-1.01913	-2.54661
H	-1.36540	0.91100	-1.69689
Si	1.92603	-1.00411	-0.00206
Li	1.81106	2.46390	0.74238

Electronic Energy = -916.9132036
Zero-point corrected electronic energy=-916.617306
Zero-point corrected Gibbs free energy=-916.642661

H	-4.13450	-1.83050	-0.97306
H	-2.81330	-0.42315	-2.53355
H	-1.08382	1.12039	-1.65827
Li	2.46367	1.76446	0.66660
C	1.75367	-1.30567	-0.03500

Electronic Energy = -665.511722939
Zero-point corrected electronic energy=-665.204622
Zero-point corrected Gibbs free energy=-665.227953

2bA-C[1]Li

C	-4.47618	0.11994	0.07255
Si	-2.80058	-0.73112	-0.10426
C	-1.46891	0.54992	0.03984
O	-0.16232	-0.02428	0.00742
C	0.89832	0.85867	-0.29211
H	0.81855	1.18173	-1.36006
C	2.19958	0.10254	-0.17920
C	3.31269	0.50406	-0.91999
C	4.53461	-0.14800	-0.77097
C	4.65111	-1.21248	0.12174
C	3.54119	-1.61813	0.86111
C	2.31942	-0.96374	0.71365
C	0.87363	2.10422	0.62006
C	-0.49872	2.74409	0.58460
C	-1.58345	1.85907	0.51084
C	-2.69547	-1.59232	-1.78081
C	-2.60267	-2.04673	1.23285
H	-4.58510	0.59108	1.05482
H	-4.62442	0.88860	-0.69356
H	-5.28205	-0.61374	-0.03523
H	3.22322	1.33141	-1.62151
H	5.39296	0.17007	-1.35487
H	5.60150	-1.72420	0.23742
H	3.62573	-2.44872	1.55534
H	1.44631	-1.27589	1.27762
H	1.15626	1.75931	1.62656
H	1.66281	2.79065	0.28991
H	-0.63205	3.73413	1.00574
H	-2.59828	2.24401	0.62719
H	-2.93421	-0.90126	-2.59665
H	-1.68081	-1.97119	-1.94358
H	-3.38546	-2.44081	-1.84265
H	-3.34509	-2.84502	1.12609
H	-2.70747	-1.60778	2.22987
H	-1.60701	-2.49776	1.16709
Li	-1.02320	2.16618	-1.41140

2bCA-C[1]Li

C	2.37781	-1.71281	-1.37271
C	1.43877	0.17004	-0.05319
O	0.89857	0.69729	1.15280
C	-0.33772	1.47638	0.97514
H	-0.61351	1.73060	2.00254
C	-1.42501	0.59944	0.40130
C	-2.18320	-0.18908	1.27083
C	-3.15377	-1.06126	0.78494
C	-3.38002	-1.15125	-0.58808
C	-2.63788	-0.36036	-1.46374
C	-1.66489	0.50934	-0.97308
C	-0.00524	2.73846	0.17080
C	1.13945	2.46414	-0.80893
C	1.52296	1.11765	-1.05198
C	2.75266	-1.60332	1.09950
C	0.48720	-2.14491	0.20842
H	1.67225	-1.56743	-2.19748
H	3.28312	-1.13278	-1.58525
H	2.65486	-2.77187	-1.34513
H	-1.99949	-0.12461	2.34122
H	-3.73291	-1.66834	1.47408
H	-4.13455	-1.83054	-0.97291
H	-2.81355	-0.42300	-2.53350
H	-1.08407	1.12049	-1.65835
H	-0.91887	3.06027	-0.35149
H	0.23105	3.55217	0.86820
H	1.24393	3.16512	-1.63030
H	1.99725	0.84816	-1.99267
H	3.71189	-1.10486	0.91105
H	2.35654	-1.25313	2.05826
H	2.94256	-2.67988	1.18286
H	0.73798	-3.21245	0.20770
H	-0.26580	-1.95993	-0.56463
H	0.04313	-1.89908	1.17729
Li	2.46367	1.76410	0.66709
C	1.75365	-1.30570	-0.03508

Electronic Energy = -916.8923209 Zero-point corrected electronic energy=-916.597788 Zero-point corrected Gibbs free energy=-916.624265	Electronic Energy = -665.502222952 Zero-point corrected electronic energy=-665.204621 Zero-point corrected Gibbs free energy=-665.22795
Silicon analogues for deprotonated C^2	Carbon analogues for deprotonated C^2
1aA-C^2Li	1aCA-C^2Li
C 2.38135 -2.26766 0.77851 Si 2.72119 -0.60302 -0.03793 C 3.62529 0.54758 1.13716 C 3.69601 -0.85018 -1.62886 C 1.03074 0.17256 -0.46394 H 0.49927 -0.47830 -1.18182 C 1.14489 1.55925 -1.03424 C 0.42082 2.58808 -0.58566 C -0.65018 2.42720 0.47143 C -0.93065 0.97491 0.71244 C -2.02344 0.23353 0.18701 C -1.95007 -1.19205 0.00661 C -3.09402 -1.95377 -0.27810 C -4.33914 -1.36686 -0.41434 C -4.42415 0.03707 -0.29410 C -3.32325 0.81095 -0.00974 O 0.29362 0.21328 0.77484 H 3.31133 -2.81211 0.97143 H 1.75075 -2.89669 0.14090 H 1.87187 -2.13440 1.73867 H 4.55381 0.09979 1.50524 H 2.98972 0.78294 1.99656 H 3.87304 1.49053 0.63982 H 4.65361 -1.33972 -1.42299 H 3.91265 0.10538 -2.11696 H 3.14669 -1.47612 -2.33958 H 1.86755 1.70388 -1.83631 H 0.58866 3.58268 -0.99453 H -1.55951 2.93555 0.13280 H -0.33410 2.95292 1.38484 H -0.97917 -1.68409 -0.04391 H -2.98130 -3.02630 -0.41907 H -5.21858 -1.95980 -0.63785 H -5.38547 0.52612 -0.43081 H -3.44159 1.88574 0.08939 Li -0.98334 -0.61524 1.88379	C 2.34338 -1.97586 0.77216 C 3.56831 0.20872 0.69055 C 3.23775 -1.14177 -1.39623 C 1.25720 -0.01156 -0.32046 H 0.62523 -0.73328 -0.87203 C 1.36477 1.24797 -1.14516 C 0.66657 2.34738 -0.85395 C -0.29858 2.38799 0.30812 C -0.58051 1.00012 0.85500 C -1.67201 0.22572 0.30190 C -1.64912 -1.20196 0.32653 C -2.73278 -1.96629 -0.08820 C -3.90867 -1.36959 -0.55588 C -3.95852 0.02744 -0.59569 C -2.88101 0.80477 -0.18562 O 0.65442 0.26284 0.94191 H 3.27958 -2.51552 0.95432 H 1.65925 -2.65265 0.24538 H 1.89515 -1.71760 1.73484 H 4.50953 -0.31170 0.90169 H 3.12784 0.52859 1.63931 H 3.80003 1.10323 0.10204 H 4.12630 -1.75435 -1.20729 H 3.55256 -0.28368 -1.99763 H 2.53748 -1.73951 -1.99169 H 2.02755 1.23463 -2.00768 H 0.79970 3.24928 -1.45139 H -1.22296 2.88270 -0.00900 H 0.12854 3.04989 1.07887 H -0.75165 -1.69610 0.68909 H -2.65660 -3.05098 -0.04981 H -4.75211 -1.96994 -0.88060 H -4.85421 0.52473 -0.96186 H -2.97796 1.88567 -0.23551 Li -1.42756 0.88896 2.82843 C 2.60889 -0.71691 -0.06335
Electronic Energy = -916.8872194 Zero-point corrected electronic energy=-916.593483 Zero-point corrected Gibbs free energy=-916.619494	Electronic Energy = -665.5281479 Zero-point corrected electronic energy=-665.224309 Zero-point corrected Gibbs free energy=-665.248781

1bA-C^{2}Li				1bCA-C^{2}Li			
C	-2.89005	0.70581	0.79501	C	-2.87026	0.87645	0.53898
C	-4.14343	0.11173	0.86657	C	-4.14448	0.32459	0.56342
C	-4.43358	-1.02982	0.11520	C	-4.37424	-0.96082	0.06616
C	-3.44295	-1.55008	-0.71480	C	-3.29944	-1.66997	-0.46465
C	-2.18614	-0.95227	-0.79520	C	-2.02045	-1.11640	-0.49918
C	-1.86909	0.18703	-0.02997	C	-1.76611	0.17043	0.01340
H	-2.69201	1.58543	1.40461	H	-2.72304	1.87280	0.95076
H	-4.90148	0.54118	1.51644	H	-4.96785	0.90160	0.97665
H	-5.41138	-1.49702	0.17472	H	-5.36933	-1.39342	0.08952
H	-3.65196	-2.43012	-1.31786	H	-3.45638	-2.66678	-0.86918
H	-1.43196	-1.35662	-1.46175	H	-1.19965	-1.67329	-0.93722
C	-0.52970	0.79060	-0.04784	C	-0.41313	0.74151	0.05757
Li	0.71969	1.14442	1.50531	Li	0.70283	1.07295	1.69722
O	0.21870	0.27881	-1.18409	O	0.45017	-0.04635	-0.82790
C	1.60025	0.47464	-0.99548	C	1.82760	0.19711	-0.69426
C	1.28465	-2.41468	-0.00392	C	2.20804	-2.25265	-0.43784
H	1.28471	-2.75845	-1.04312	H	2.56040	-2.30809	-1.47380
H	1.63992	-3.23153	0.63196	H	2.69290	-3.05506	0.12879
H	0.24907	-2.17553	0.26232	H	1.12817	-2.41921	-0.43873
C	2.35006	-0.36136	2.02341	C	2.06813	-0.87708	1.62917
H	1.39207	-0.54989	2.52914	H	0.98219	-1.03092	1.68666
H	3.07882	-0.98930	2.54623	H	2.54136	-1.68706	2.19352
H	2.69033	0.67044	2.20361	H	2.38305	0.04724	2.14822
C	4.13621	-1.14684	-0.29677	C	4.05975	-0.67046	0.13343
H	4.71910	-0.22580	-0.18526	H	4.36383	0.23105	0.67584
H	4.60016	-1.91321	0.33268	H	4.57259	-1.52097	0.59520
H	4.22223	-1.47227	-1.33837	H	4.42002	-0.58509	-0.89802
C	1.91645	1.88433	-0.57009	C	2.12861	1.63604	-0.32128
H	2.96327	2.18849	-0.57468	H	3.17494	1.91910	-0.22819
C	-0.50286	2.32043	-0.21511	C	-0.28334	2.18575	-0.43310
H	-0.99777	2.64591	-1.14789	H	-0.59021	2.29840	-1.49026
H	-1.03256	2.83189	0.60083	H	-0.91027	2.87148	0.14886
C	0.94976	2.76073	-0.23853	C	1.16903	2.57768	-0.29631
H	1.21043	3.79148	-0.00358	H	1.44477	3.62465	-0.17526
H	2.07922	0.30490	-1.97383	C	2.54223	-0.88590	0.17004
Si	2.33170	-0.87895	0.17470	H	2.25088	0.06780	-1.70523
Electronic Energy = -916.8752684 Zero-point corrected electronic energy=-916.581233 Zero-point corrected Gibbs free energy=-916.606297				Electronic Energy = -665.483070016 Zero-point corrected electronic energy=-665.177938 Zero-point corrected Gibbs free energy=-665.201801			
2aA-C^{2}Li				2aCA-C^{2}Li			
C	3.81591	-0.86782	-0.83513	C	3.72687	-0.92311	-0.69003
C	0.87603	-0.94039	-1.74537	C	1.36393	-0.93029	-1.52193
C	1.82265	-2.57791	0.73414	C	2.01294	-2.30681	0.47484
C	1.73872	0.51687	0.90431	C	1.95489	0.18414	0.69198

H	2.32585	0.34360	1.81787	H	2.51175	-0.02185	1.61855
C	2.18420	1.79816	0.26772	C	2.37953	1.53881	0.19425
C	1.32648	2.70526	-0.20632	C	1.52411	2.52107	-0.08749
C	-0.16954	2.52454	-0.16089	C	0.03123	2.36445	-0.00331
C	-0.54644	1.19515	0.41412	C	-0.35635	0.96112	0.33069
C	-1.64744	0.40079	0.11108	C	-1.55398	0.31618	0.05386
C	-1.83910	-0.91595	0.68868	C	-1.81341	-1.05718	0.44646
C	-3.02771	-1.63335	0.47971	C	-3.08433	-1.63080	0.27928
C	-4.07144	-1.12174	-0.26895	C	-4.14807	-0.92090	-0.24537
C	-3.89260	0.15059	-0.86504	C	-3.90996	0.41329	-0.65646
C	-2.74781	0.88700	-0.69227	C	-2.68531	1.01642	-0.51988
O	0.37444	0.64224	1.35545	O	0.58427	0.21074	1.10928
H	4.10051	-1.77008	-1.38687	H	4.00132	-1.83857	-1.22437
H	4.50727	-0.76352	0.00831	H	4.38800	-0.83558	0.18154
H	3.95858	-0.01094	-1.50123	H	3.91938	-0.07705	-1.35647
H	1.20562	-1.67317	-2.49068	H	1.67609	-1.70904	-2.22719
H	0.89366	0.05160	-2.20967	H	1.45134	0.03970	-2.02288
H	-0.15787	-1.16524	-1.46925	H	0.31087	-1.09403	-1.27719
H	2.00865	-3.44928	0.09712	H	2.15665	-3.15865	-0.19801
H	0.81699	-2.68406	1.15010	H	0.99529	-2.35981	0.87086
H	2.54034	-2.61029	1.56089	H	2.71354	-2.41475	1.31167
H	3.25739	1.95841	0.18938	H	3.44982	1.70503	0.10723
H	1.70310	3.62513	-0.64767	H	1.90458	3.49244	-0.39561
H	-0.55366	2.59751	-1.18804	H	-0.39480	2.63479	-0.97922
H	-0.60920	3.38397	0.37596	H	-0.35875	3.12155	0.70268
H	-0.98854	-1.42959	1.13281	H	-0.97681	-1.70530	0.69686
H	-3.10869	-2.62954	0.90942	H	-3.21601	-2.67395	0.55869
H	-4.98626	-1.68254	-0.41929	H	-5.12514	-1.37388	-0.36470
H	-4.68594	0.56353	-1.48375	H	-4.72202	0.98533	-1.09947
H	-2.66050	1.85995	-1.16656	H	-2.55506	2.04283	-0.84961
Li	-1.26847	0.49864	2.20008	C	2.25049	-0.99046	-0.27431
Si	2.02223	-0.99118	-0.26267	Li	-0.98654	0.07314	2.07896
Electronic Energy = -916.8862627 Zero-point corrected electronic energy=-916.591943 Zero-point corrected Gibbs free energy=-916.61691				Electronic Energy = -665.4961208 Zero-point corrected electronic energy=-665.190412 Zero-point corrected Gibbs free energy=-665.213894			
2bA-C^{2}Li				2bCA-C^{2}Li			
C	3.36364	0.86570	0.06617	C	3.07635	0.93999	-0.05213
C	4.58188	0.21695	0.22947	C	4.33444	0.36238	0.07293
C	4.66290	-1.17470	0.15168	C	4.47943	-1.02579	0.10512
C	3.49591	-1.89784	-0.08780	C	3.33627	-1.81766	0.01491
C	2.27210	-1.25113	-0.24654	C	2.07322	-1.24182	-0.10559
C	2.17307	0.15159	-0.18156	C	1.90913	0.15499	-0.15076
H	3.33893	1.95185	0.11839	H	2.99997	2.02468	-0.08797
H	5.47739	0.80265	0.42028	H	5.21041	1.00180	0.14473
H	5.61452	-1.68098	0.27820	H	5.46164	-1.47723	0.20215
H	3.53483	-2.98261	-0.14653	H	3.42552	-2.90057	0.04502
H	1.37087	-1.82682	-0.42630	H	1.19203	-1.87096	-0.16685

C	0.89626	0.85003	-0.39832	C	0.58744	0.77604	-0.33355
Li	0.26348	2.09209	-1.86952	Li	-0.15371	1.85043	-1.88799
O	-0.19678	-0.10174	-0.23804	O	-0.44432	-0.20064	-0.02219
C	-1.42000	0.37134	-0.74275	C	-1.69519	0.14439	-0.54053
C	-4.44224	-0.27260	-0.61375	C	-4.10867	-0.59515	-0.63699
H	-4.45657	-0.38533	-1.70314	H	-4.02118	-0.72297	-1.72278
H	-5.21669	-0.92977	-0.20447	H	-4.83195	-1.33247	-0.27368
H	-4.72605	0.75731	-0.37325	H	-4.52916	0.39580	-0.43807
C	-2.70128	-0.36184	1.94617	C	-2.89841	-0.56554	1.56567
H	-2.93181	0.68873	2.15126	H	-3.29303	0.43455	1.77618
H	-3.41971	-0.98170	2.49229	H	-3.58627	-1.29814	2.00175
H	-1.69944	-0.57015	2.33342	H	-1.92590	-0.66212	2.05616
C	-2.32511	-2.50646	-0.26590	C	-2.29183	-2.24798	-0.18867
H	-1.31599	-2.72347	0.09657	H	-1.34767	-2.44173	0.32495
H	-3.02473	-3.19385	0.22036	H	-3.04450	-2.95497	0.17657
H	-2.34856	-2.70288	-1.34265	H	-2.14196	-2.43233	-1.25920
C	-1.65362	1.82725	-0.43383	C	-2.00702	1.61064	-0.28624
H	-2.61679	2.25113	-0.71900	H	-3.00651	1.96650	-0.52828
C	0.58947	1.96614	0.61445	C	0.28724	1.95895	0.60032
H	0.57053	1.58288	1.65169	H	0.35526	1.67123	1.66594
H	1.34899	2.75751	0.59233	H	0.99199	2.78797	0.45973
C	-0.76397	2.55323	0.27166	C	-1.11862	2.43155	0.30146
H	-1.01619	3.56467	0.58645	H	-1.41298	3.44917	0.55597
H	-1.48582	0.20070	-1.84293	C	-2.75993	-0.80881	0.05939
Si	-2.75628	-0.71915	0.10535	H	-1.70319	-0.04134	-1.64278
Electronic Energy = -916.8728438 Zero-point corrected electronic energy=-916.580117 Zero-point corrected Gibbs free energy=-916.606573				Electronic Energy = -665.4833809 Zero-point corrected electronic energy=-665.178263 Zero-point corrected Gibbs free energy= -665.202486			
A Intermediates (Anionic)							
Silicon analogues for deprotonated C[1]				Carbon Analogues for deprotonated C[1]			
1-Anionic				1C-Anionic			
C	-1.97134	-2.23694	-0.38633	C	-2.03531	-2.02383	-0.40111
C	-3.83420	0.00897	-1.04167	C	-3.58067	-0.09415	-0.73019
C	-3.08666	-0.51244	1.87568	C	-2.98855	-0.84827	1.57634
C	-1.00521	0.73788	0.04761	C	-1.27876	0.30823	0.16395
C	-0.52731	1.54881	1.08562	C	-0.92581	1.23120	1.13089
C	0.48971	2.47505	0.95604	C	-0.07535	2.32226	0.91094
C	1.10370	2.62118	-0.40632	C	0.41077	2.50187	-0.49526
C	0.98776	1.26998	-1.13795	C	0.51521	1.10875	-1.15449
H	1.31856	1.37757	-2.18153	H	0.76960	1.20493	-2.22070
C	1.81443	0.15348	-0.50851	C	1.56352	0.20639	-0.51217
C	1.41958	-1.17129	-0.71733	C	1.45352	-1.17822	-0.67002
C	2.18065	-2.23457	-0.23247	C	2.43383	-2.04062	-0.17649
C	3.35373	-1.98734	0.48052	C	3.54146	-1.52566	0.49739
C	3.74826	-0.67025	0.71002	C	3.65231	-0.14820	0.67777
C	2.97737	0.39025	0.22801	C	2.66348	0.70984	0.18574
O	-0.37789	0.90206	-1.23395	O	-0.76075	0.49206	-1.15000

H	-2.85785	-2.87858	-0.29534
H	-1.17515	-2.64446	0.24626
H	-1.63395	-2.28535	-1.42877
H	-4.61347	-0.76479	-1.04992
H	-3.46525	0.13560	-2.06602
H	-4.28473	0.95878	-0.73323
H	-3.94185	-1.19811	1.91123
H	-3.42806	0.47469	2.20524
H	-2.33317	-0.86696	2.58691
H	-0.98125	1.39667	2.06606
H	0.86742	3.03399	1.80541
H	2.15468	2.94390	-0.36982
H	0.59005	3.35459	-1.05131
H	0.49826	-1.34993	-1.26171
H	1.84931	-3.25611	-0.40267
H	3.94956	-2.81282	0.86199
H	4.65232	-0.46331	1.27735
H	3.27933	1.40986	0.44459
Si	-2.38032	-0.43845	0.11353

Electronic Energy = -909.3772165
Zero-point corrected electronic energy=-909.086622
Zero-point corrected Gibbs free energy=-909.11235

H	-2.90010	-2.70162	-0.44746
H	-1.26249	-2.47658	0.23009
H	-1.63223	-1.91234	-1.41317
H	-4.42708	-0.79542	-0.78948
H	-3.20406	0.08700	-1.74195
H	-3.93916	0.85898	-0.32647
H	-3.80920	-1.57726	1.56192
H	-3.37369	0.09091	1.98747
H	-2.20343	-1.21919	2.24483
H	-1.30414	1.05972	2.13793
H	0.35186	2.88515	1.73334
H	1.37902	3.02164	-0.55432
H	-0.27191	3.07852	-1.14512
H	0.58199	-1.56588	-1.18732
H	2.32602	-3.11444	-0.30912
H	4.30692	-2.19337	0.88545
H	4.50455	0.26382	1.21271
H	2.74436	1.77668	0.36328
C	-2.44144	-0.64755	0.15974

Electronic Energy = -657.967869869
Zero-point corrected electronic energy=-657.666656
Zero-point corrected Gibbs free energy=-657.690418

2-Anionic

C	-2.44814	-0.64774	-0.97198
C	-3.69132	-1.26473	-1.10073
C	-4.65132	-1.13739	-0.09588
C	-4.35403	-0.38914	1.04337
C	-3.10799	0.22294	1.17084
C	-2.14114	0.10401	0.16807
H	-1.68580	-0.74977	-1.73842
H	-3.91405	-1.84946	-1.98973
H	-5.62040	-1.61827	-0.19863
H	-5.09168	-0.28615	1.83509
H	-2.87414	0.80215	2.06175
C	-0.82298	0.82075	0.27607
H	-0.55881	0.95396	1.34007
O	0.16493	0.03225	-0.35710
C	1.48297	0.57875	-0.21285
Si	2.78286	-0.63994	0.09317
C	2.94562	-1.94647	-1.28883
H	3.24897	-1.47183	-2.22837
H	3.67349	-2.72906	-1.03754
H	1.97355	-2.42428	-1.45748
C	2.53439	-1.68817	1.67016
H	1.53369	-2.13585	1.65532
H	3.26998	-2.49899	1.75445

2C-Anionic

C	2.23872	-0.36903	1.05595
C	3.52423	-0.88598	1.20534
C	4.41340	-0.89386	0.12972
C	4.00124	-0.38177	-1.10217
C	2.71381	0.13189	-1.24945
C	1.81599	0.14761	-0.17749
H	1.53159	-0.37437	1.88027
H	3.83622	-1.28678	2.16678
H	5.41508	-1.29810	0.24859
H	4.68164	-0.38785	-1.94998
H	2.39154	0.52657	-2.21080
C	0.45256	0.75325	-0.30519
H	0.17790	0.84449	-1.36989
O	-0.46647	-0.11201	0.35113
C	-1.81314	0.31987	0.24195
C	-4.19304	-0.36823	-0.14536
H	-4.34578	0.35209	-0.95656
H	-4.85023	-1.22925	-0.32440
H	-4.49172	0.10846	0.79531
C	-2.61207	-1.92295	0.99828
H	-2.95113	-1.53476	1.96504
H	-3.21285	-2.80787	0.74047
H	-1.56597	-2.22741	1.10215

H	2.60241	-1.05833	2.56394
C	4.47260	0.21772	0.24488
H	4.49236	0.89822	1.10292
H	5.26579	-0.52732	0.38130
H	4.70118	0.79841	-0.65531
C	1.57072	1.97792	-0.22052
H	2.56981	2.39993	-0.09624
C	-0.87784	2.21897	-0.38470
H	-1.27417	2.06205	-1.40511
H	-1.62710	2.82898	0.14506
C	0.49272	2.83233	-0.33515
H	0.60978	3.90835	-0.25715

Electronic Energy = -909.3788602
Zero-point corrected electronic energy=-909.088729
Zero-point corrected Gibbs free energy=-909.115198

C	-2.35310	-1.45318	-1.44196
H	-1.29369	-1.73129	-1.43390
H	-2.94769	-2.35326	-1.66079
H	-2.51050	-0.72508	-2.24578
C	-2.04436	1.67776	0.15425
H	-3.07265	1.99751	-0.01205
C	0.36323	2.16202	0.34238
H	0.74117	2.02118	1.37559
H	1.08207	2.83082	-0.15687
C	-1.04469	2.65513	0.24402
H	-1.25537	3.69528	0.02237
C	-2.73412	-0.82659	-0.08104

Electronic Energy = -657.970269151
Zero-point corrected electronic energy=-657.669714
Zero-point corrected Gibbs free energy=-657.694105

Silicon analogues for deprotonated C^2

1-Anionic

C	2.30313	-2.48023	0.08987
C	3.16144	-0.04020	1.77898
C	4.29448	-0.42181	-1.06179
C	1.30417	0.32531	-0.65476
H	1.07809	-0.01857	-1.68480
C	1.56638	1.80878	-0.67236
C	0.68685	2.67778	-0.16540
C	-0.66900	2.23894	0.32874
C	-0.91680	0.80002	0.01994
C	-2.14438	0.16652	0.00626
C	-2.27708	-1.27239	-0.07769
C	-3.51117	-1.88867	-0.14223
C	-4.71866	-1.16578	-0.11023
C	-4.61874	0.22940	0.01955
C	-3.40074	0.88074	0.09199
O	0.23448	-0.00620	0.21112
H	3.08082	-3.09252	0.55960
H	2.12583	-2.86346	-0.92072
H	1.37330	-2.59175	0.65626
H	3.97897	-0.60542	2.24049
H	2.26660	-0.13849	2.40105
H	3.43681	1.01941	1.75780
H	5.13306	-1.03238	-0.70807
H	4.62206	0.62349	-1.06859
H	4.07863	-0.71368	-2.09544
H	2.51506	2.15434	-1.08577
H	0.93136	3.73975	-0.12709
H	-1.42681	2.86539	-0.16029
H	-0.74113	2.48575	1.41423

Carbon analogues for deprotonated C^2

1-Anionic

C	-2.18654	-2.20459	-0.21932
C	-3.34180	-0.25035	-1.27380
C	-3.76276	-0.82562	1.13418
C	-1.51872	0.10429	0.44004
H	-1.11676	-0.30797	1.38652
C	-1.88393	1.55906	0.64962
C	-1.07074	2.54144	0.25278
C	0.28527	2.26546	-0.34955
C	0.59666	0.80901	-0.30637
C	1.82559	0.20873	-0.14684
C	1.98623	-1.23221	-0.10892
C	3.21668	-1.82474	0.09300
C	4.39929	-1.07827	0.25683
C	4.27800	0.32022	0.18441
C	3.06503	0.95145	-0.01843
O	-0.52976	-0.00659	-0.56122
H	-3.01029	-2.87755	-0.48927
H	-1.70544	-2.59420	0.68603
H	-1.44310	-2.20645	-1.01977
H	-4.13519	-0.92523	-1.61996
H	-2.57815	-0.16822	-2.05218
H	-3.77864	0.74286	-1.12117
H	-4.55821	-1.53502	0.87424
H	-4.23226	0.14994	1.29713
H	-3.31607	-1.15244	2.08108
H	-2.83522	1.79212	1.12529
H	-1.37871	3.58137	0.37060
H	1.03458	2.82983	0.22203
H	0.29879	2.70947	-1.37051

H	-1.36921	-1.86780	-0.10306
H	-3.54349	-2.97635	-0.21571
H	-5.68138	-1.66439	-0.16095
H	-5.52913	0.82701	0.07764
H	-3.39064	1.96146	0.21113
Si	2.77329	-0.65804	0.04416

Electronic Energy = -909.3613508
Zero-point corrected electronic energy=-909.072772
Zero-point corrected Gibbs free energy=-909.098967

H	1.10021	-1.84788	-0.23520
H	3.26652	-2.91400	0.12180
H	5.36016	-1.55896	0.40983
H	5.17143	0.93876	0.27942
H	3.04427	2.03649	-0.08832
C	-2.71324	-0.78391	0.01771

Electronic Energy = -657.9746556
Zero-point corrected electronic energy=-657.674256
Zero-point corrected Gibbs free energy=-657.697221

2-Anionic

H	-3.16548	-2.44892	-1.14782
C	-3.02185	-1.49618	-0.63659
C	-1.89126	-0.75854	-0.93188
H	-1.18556	-1.11651	-1.67515
C	-1.61515	0.51294	-0.29085
C	-0.44873	1.21021	-0.50809
C	-2.66279	0.97051	0.60239
H	-2.57231	1.94598	1.07365
C	-3.77778	0.20062	0.87529
H	-4.52000	0.59661	1.56916
C	-3.99111	-1.05764	0.28419
H	-4.87367	-1.64811	0.50745
O	0.46723	0.71648	-1.46656
C	-0.08250	2.54137	0.06100
C	1.41162	2.68755	0.21366
H	-0.53888	2.65857	1.05469
H	-0.45339	3.40664	-0.53208
C	2.25656	1.74244	-0.21114
H	1.79544	3.59280	0.68467
C	1.75822	0.50631	-0.90727
H	3.33178	1.84377	-0.06449
Si	1.83708	-1.02520	0.24637
C	3.64759	-1.14647	0.81975
C	1.44948	-2.58686	-0.74144
C	0.73535	-0.92170	1.76339
H	4.33939	-1.13279	-0.03094
H	3.81681	-2.07689	1.37429
H	3.90562	-0.31030	1.47887
H	0.85468	0.04845	2.25812
H	0.99361	-1.71495	2.47701
H	-0.31723	-1.01996	1.47862
H	2.04198	-2.63255	-1.66205
H	0.38912	-2.60670	-1.00871
H	1.67004	-3.48089	-0.14652
H	2.42519	0.28932	-1.75988

Electronic Energy = -909.3655671

2-Anionic

C	-2.68061	1.03601	0.39798
C	-3.87930	0.39591	0.64835
C	-4.10998	-0.94449	0.28993
C	-3.06262	-1.61057	-0.37125
C	-1.84777	-1.00693	-0.63519
C	-1.56006	0.35417	-0.22490
H	-2.57981	2.08225	0.67574
H	-4.67575	0.96347	1.13111
H	-5.05967	-1.43089	0.48777
H	-3.20951	-2.63971	-0.70115
H	-1.08159	-1.55103	-1.17771
C	-0.33139	0.94459	-0.41234
O	0.62850	0.26200	-1.20688
C	1.93720	0.21925	-0.67761
C	1.94969	-2.27663	-0.57635
H	2.67586	-2.34747	-1.39693
H	2.05784	-3.16850	0.05328
H	0.94466	-2.27285	-1.00466
C	1.23496	-1.00991	1.45686
H	0.19257	-1.11542	1.14335
H	1.49442	-1.84859	2.11804
H	1.32083	-0.07757	2.02559
C	3.63347	-0.99310	0.74013
H	3.80866	-0.18493	1.45800
H	3.86808	-1.94125	1.23948
H	4.33657	-0.87108	-0.09512
C	2.35219	1.54449	-0.08664
H	3.41445	1.69216	0.10081
C	0.00974	2.36427	-0.11826
H	-0.29232	3.08479	-0.91342
H	-0.52402	2.69220	0.78396
C	1.48483	2.53665	0.12089
H	1.84187	3.50651	0.46898
C	2.17858	-1.00665	0.25076
H	2.58548	0.04962	-1.55619

Zero-point corrected electronic energy = -909.076048 Zero-point corrected Gibbs free energy = -909.121585	Electronic Energy = -657.974192 Zero-point corrected electronic energy=-657.673295 Zero-point corrected Gibbs free energy=-657.696678

Deprotonation Transition States							
TS for Deprotonation of C^1				TS for Deprotonation of C^2			
1a-TS- C^1				1a-TS- C^2			
C	0.20211	-1.54862	-1.57727	C	-2.63858	1.78269	-1.75562
C	-0.85713	-2.34699	-1.80423	Si	-3.20189	0.39624	-0.60520
C	0.52333	-0.92470	-0.30281	C	-3.69734	1.09399	1.06385
H	0.87188	-1.29589	-2.39939	C	-4.60382	-0.57216	-1.40159
O	-0.38186	-1.34503	0.80154	C	-1.70240	-0.75916	-0.33370
H	0.37356	0.48159	-0.36163	H	-1.40084	-1.22513	-1.28747
Si	2.24160	-1.27175	0.36901	C	-2.00456	-1.82914	0.66767
C	-1.79380	-2.70946	-0.68379	C	-1.36966	-1.93045	1.83705
H	-1.04656	-2.75263	-2.79334	C	-0.21697	-1.02445	2.18967
C	-1.73757	-1.69907	0.46350	C	0.41067	-0.41414	0.95377
H	-1.54401	-3.69835	-0.27654	H	0.90940	0.81069	1.43191
H	-2.83080	-2.77381	-1.03581	C	1.36802	-1.21765	0.16831
H	-2.10683	-2.17959	1.37677	C	1.41850	-1.14159	-1.23838
C	-2.54664	-0.42609	0.27018	C	2.40580	-1.79832	-1.97004
C	2.43147	-3.05726	0.93614	C	3.38402	-2.55192	-1.32617
C	2.41921	-0.15252	1.89315	C	3.35585	-2.63290	0.06737
C	3.52274	-0.88997	-0.95939	C	2.37155	-1.98008	0.80012
H	1.67955	-3.29638	1.69463	O	-0.65909	0.12217	0.11686
H	3.42274	-3.24246	1.36402	H	-3.48698	2.40236	-2.06369
H	2.28937	-3.74210	0.09361	H	-2.16853	1.38550	-2.66155
H	1.72533	-0.48104	2.67894	H	-1.92248	2.44971	-1.26114
H	2.22818	0.90353	1.66182	H	-4.46999	1.86274	0.96259
H	3.42407	-0.20874	2.32422	H	-2.82924	1.54275	1.55903
H	3.61359	-1.74579	-1.63691	H	-4.08038	0.30495	1.71809
H	4.50833	-0.70557	-0.51925	H	-5.45969	0.08117	-1.60026
H	3.25030	-0.01505	-1.55620	H	-4.94876	-1.38032	-0.74901
C	-3.00878	0.23394	1.41749	H	-4.29263	-1.01401	-2.35381
C	-2.78290	0.15418	-0.97930	H	-2.79666	-2.52610	0.39917
C	-3.68851	1.44865	1.32436	H	-1.66625	-2.70108	2.54512
C	-3.92161	2.01424	0.07244	H	0.53260	-1.58213	2.75856
C	-3.47070	1.36220	-1.07431	H	-0.55993	-0.21523	2.85509
H	-2.40924	-0.33408	-1.87448	H	0.66703	-0.56429	-1.77127
H	-3.64073	1.80574	-2.05053	H	2.40559	-1.72021	-3.05389
H	-4.44781	2.96003	-0.00911	H	4.15326	-3.06432	-1.89440
H	-2.85966	-0.22784	2.39353	H	4.11278	-3.20975	0.59147
H	-4.04577	1.94165	2.22342	H	2.39165	-2.05117	1.88354
C	-0.01685	1.97376	-0.25641	C	1.94992	3.06588	0.75898
H	-0.23724	2.00113	-1.33471	H	1.22822	3.52106	0.04342
H	-0.97320	2.29571	0.20480	H	2.47189	3.94345	1.16969
C	1.06806	3.01006	0.06290	C	2.96746	2.24028	-0.04333

H	0.75934	4.03292	-0.21119	H	2.48859	1.37629	-0.53547
H	1.26134	3.05378	1.14895	H	3.67383	1.79043	0.66504
C	2.39373	2.71834	-0.64036	C	3.71699	3.06007	-1.09027
H	2.77171	1.74296	-0.31084	H	4.26120	3.88482	-0.61876
H	2.20818	2.62336	-1.71941	H	4.43793	2.44814	-1.63906
C	3.45675	3.78554	-0.38880	H	3.02431	3.49637	-1.81910
H	3.66750	3.87903	0.68264	Li	0.31455	1.63715	0.07264
H	4.39746	3.54984	-0.89563	C	1.22746	2.23323	1.83577
H	3.11875	4.76441	-0.74521	H	0.46339	2.83387	2.34720
Li	-0.30477	0.51697	1.22114	H	1.95845	1.93813	2.59815
One imaginary frequency: -1344.15 cm^{-1} Electronic Energy = -1075.233501 Zero-point corrected electronic energy=-1074.809896 Zero-point corrected Gibbs free energy=-1074.839744				One imaginary frequency: -1263.15 cm^{-1} Electronic Energy = -1075.229149 Zero-point corrected electronic energy=-1074.806487 Zero-point corrected Gibbs free energy=-1074.83806			
1b-TS- C^1				1b-TS- C^2			
C	3.31841	-2.37984	-0.49576	C	4.69743	0.67870	1.21135
Si	1.70977	-1.51529	-0.96263	Si	3.02465	0.74564	0.34624
C	0.58481	-2.71269	-1.90100	C	3.27446	1.06571	-1.48713
C	2.07742	-0.07554	-2.12681	C	1.96420	2.06576	1.20228
C	0.90808	-0.88633	0.61394	C	2.19193	-0.96615	0.65745
H	1.52915	0.18948	1.23416	H	2.56479	-1.29023	1.64199
C	0.74555	-1.83647	1.71180	C	2.64428	-1.96048	-0.35828
C	-0.39882	-2.03605	2.39202	C	1.81852	-2.59727	-1.18740
C	-1.68557	-1.38912	1.95162	C	0.33204	-2.40921	-1.14808
C	-1.56632	-0.94039	0.49638	C	-0.10170	-1.21832	-0.31203
H	-1.50002	-1.82959	-0.14515	H	-0.12869	0.02073	-1.02106
C	-2.69078	-0.05527	0.02381	C	-1.47577	-1.28267	0.20921
C	-3.44202	-0.39031	-1.10338	C	-2.52661	-1.70099	-0.63750
C	-4.46136	0.44804	-1.55357	C	-3.85282	-1.59255	-0.24671
C	-4.73314	1.63926	-0.88435	C	-4.19412	-1.04870	0.99702
C	-3.98527	1.98655	0.24091	C	-3.17579	-0.64573	1.85253
C	-2.97523	1.14102	0.69276	C	-1.83570	-0.76579	1.47351
O	-0.35619	-0.18641	0.32238	O	0.76859	-0.91141	0.82675
H	3.89862	-2.62957	-1.39028	H	5.26901	1.59263	1.01862
H	3.93756	-1.73682	0.13908	H	4.58235	0.57510	2.29531
H	3.12625	-3.31017	0.04831	H	5.29655	-0.16575	0.85375
H	1.09045	-3.12281	-2.78239	H	3.38569	2.13440	-1.69818
H	0.27771	-3.54917	-1.26435	H	4.17944	0.55420	-1.83143
H	-0.31829	-2.19747	-2.24870	H	2.42978	0.68771	-2.06947
H	2.44074	-0.45125	-3.08960	H	2.60144	2.88036	1.56185
H	1.17580	0.51555	-2.32551	H	1.22862	2.52731	0.53421
H	2.84383	0.58946	-1.71601	H	1.45927	1.65629	2.08811
H	1.64921	-2.36456	2.01459	H	3.71875	-2.13190	-0.40818
H	-0.42405	-2.71153	3.24165	H	2.21677	-3.30382	-1.91122
H	-2.52465	-2.09247	2.02702	H	-0.03229	-2.27024	-2.17463
H	-1.94826	-0.53027	2.58407	H	-0.13000	-3.34296	-0.78643
H	-3.22437	-1.31467	-1.63253	H	-2.29269	-2.10361	-1.61882

H	-5.03979	0.17232	-2.42982
H	-5.52457	2.29398	-1.23515
H	-4.19687	2.91026	0.77079
H	-2.41601	1.40620	1.58876
Li	0.29987	1.43370	0.79434
C	2.04751	1.41239	1.95602
C	3.09598	1.99101	1.00259
H	2.51510	0.80733	2.74180
H	1.55614	2.24316	2.50032
H	3.59965	1.16695	0.47012
H	3.89639	2.54683	1.51498
C	2.46868	2.92201	-0.04003
H	1.72520	2.36339	-0.63813
C	3.47756	3.53597	-1.00810
H	1.92550	3.72543	0.48035
H	4.02015	2.75243	-1.54744
H	4.21430	4.13382	-0.46243
H	2.99529	4.18252	-1.74674

One imaginary frequency: -1258.06 cm^{-1}
Electronic Energy = -1075.240418
Zero-point corrected electronic energy=-1074.816298
Zero-point corrected Gibbs free energy=-1074.846276

H	-4.63485	-1.92579	-0.92313
H	-5.23391	-0.95496	1.29168
H	-3.41610	-0.24948	2.83535
H	-1.05882	-0.52800	2.19809
Li	-0.20614	0.75794	0.51756
C	-0.28089	1.47451	-1.46441
H	0.67562	1.98974	-1.62359
C	-1.29634	2.44802	-0.81922
H	-0.65251	1.22278	-2.46705
H	-1.21971	3.46091	-1.24543
H	-1.09545	2.62006	0.26393
C	-2.75063	1.98848	-0.93946
H	-3.00724	1.93932	-2.00551
C	-3.73021	2.90141	-0.20644
H	-2.85101	0.96647	-0.55645
H	-3.67308	3.92963	-0.58045
H	-3.50926	2.92369	0.86720
H	-4.76145	2.55562	-0.32328

One imaginary frequency: -1379.54 cm^{-1}
Electronic Energy = -1075.221758
Zero-point corrected electronic energy=-1074.798484
Zero-point corrected Gibbs free energy=-1074.827632

2a-TS- C^1

C	-0.21144	0.99290	1.79424
C	0.38543	2.19908	1.74685
C	-0.56625	0.20356	0.62530
H	-0.49194	0.56511	2.75684
O	-0.20794	0.86871	-0.63638
H	-1.90816	0.30577	0.45767
Si	-0.31556	-1.65249	0.56974
C	0.82290	2.78544	0.43070
H	0.57479	2.76070	2.65666
C	0.96252	1.70090	-0.63949
H	1.77873	3.31517	0.52810
H	0.09492	3.52529	0.06878
H	0.94638	2.17024	-1.63001
C	2.21646	0.84528	-0.56927
C	1.39639	-2.36678	0.88996
C	-0.85348	-2.12178	-1.18926
C	-1.52584	-2.36844	1.82769
H	2.10862	-2.07257	0.11273
H	1.35558	-3.46185	0.92431
H	1.78634	-2.01090	1.84954
H	-0.17044	-1.67909	-1.92381
H	-1.88166	-1.79645	-1.40760
H	-0.84058	-3.20589	-1.33956
H	-1.18981	-2.17033	2.85129

2a-TS- C^2

C	3.84892	-2.30851	-0.31150
Si	2.52350	-0.98675	-0.59659
C	3.19826	0.65037	0.02174
C	2.10714	-0.96810	-2.43245
C	1.01946	-1.68095	0.40289
H	1.02154	-2.74908	0.12997
C	1.24313	-1.58019	1.88080
C	0.39354	-0.98115	2.71872
C	-0.89194	-0.37147	2.21825
C	-0.83819	-0.05694	0.73625
H	-2.08266	0.06675	0.02465
C	-0.15856	1.19241	0.31658
C	-0.08034	1.47084	-1.06217
C	0.43847	2.67264	-1.53217
C	0.89315	3.64129	-0.63566
C	0.81955	3.38490	0.73335
C	0.30322	2.17939	1.20345
O	-0.29246	-1.22182	0.02304
H	4.74504	-2.06943	-0.89429
H	3.50836	-3.30275	-0.62008
H	4.14958	-2.36370	0.74020
H	4.24590	0.75131	-0.28333
H	3.15658	0.69186	1.11550
H	2.64024	1.50624	-0.36592

H	-1.61926	-3.45380	1.71493	H	3.02891	-0.93281	-3.02285
H	-2.51912	-1.92267	1.70755	H	1.50071	-0.10011	-2.70022
C	2.56741	0.10627	-1.70499	H	1.56152	-1.87369	-2.71938
C	3.03257	0.76610	0.56015	H	2.16705	-2.02021	2.25279
C	3.70929	-0.69030	-1.71914	H	0.61569	-0.95393	3.78361
C	4.52322	-0.75501	-0.58785	H	-1.14255	0.53569	2.77773
C	4.18079	-0.02659	0.54890	H	-1.72001	-1.06686	2.42812
H	2.76329	1.31528	1.45708	H	-0.45445	0.73265	-1.76695
H	4.80574	-0.07735	1.43534	H	0.48092	2.85916	-2.60193
H	5.41698	-1.37112	-0.59336	H	1.29707	4.58090	-0.99894
H	1.93813	0.16457	-2.59120	H	1.17958	4.12461	1.44279
H	3.96827	-1.25283	-2.61095	H	0.27738	2.00102	2.27426
C	-3.33946	0.82121	-0.01404	C	-4.23043	-1.10889	-0.24490
H	-3.81027	0.68605	0.96665	H	-3.87120	-1.54185	0.71256
C	-4.21747	0.15166	-1.07336	H	-5.26889	-0.81626	-0.02384
H	-5.08816	0.77695	-1.34297	C	-4.28697	-2.20836	-1.31625
H	-3.68738	0.04207	-2.05421	H	-3.30299	-2.60932	-1.61973
C	-4.71220	-1.23243	-0.65467	H	-4.73168	-1.81105	-2.23285
H	-3.87701	-1.88654	-0.38206	Li	-1.97390	-1.49660	-0.54460
H	-5.35362	-1.14289	0.22785	C	-3.37209	0.10482	-0.63212
Li	-1.85255	0.53987	-1.33905	H	-3.49239	0.31076	-1.70508
C	-3.17420	2.31818	-0.29222	H	-4.87409	-3.07031	-0.98917
H	-2.64982	2.52715	-1.24832	C	-3.76322	1.33740	0.17763
H	-2.57315	2.80078	0.48637	H	-3.55744	1.17713	1.24711
H	-4.12968	2.86175	-0.37792	H	-3.17511	2.21012	-0.12642
H	-5.28861	-1.72257	-1.44491	H	-4.82874	1.59498	0.08867
One imaginary frequency: -1248.82 cm^{-1} Electronic Energy = Zero-point corrected electronic energy= Zero-point corrected Gibbs free energy=				One imaginary frequency: -1247.31 cm^{-1} Electronic Energy = -1075.224303 Zero-point corrected electronic energy=-1074.800674 Zero-point corrected Gibbs free energy=-1074.830277			
2b-TS- C^1				2b-TS- C^2			
C	-1.24400	-0.93357	1.88918	C	2.82459	1.03657	-1.96171
C	-0.20760	-1.26937	2.68055	Si	2.86663	-0.06060	-0.43089
C	-1.11873	-0.46709	0.50945	C	2.77380	0.94979	1.14788
H	-2.25803	-0.97269	2.28727	C	4.47628	-1.04910	-0.43335
O	0.27399	-0.55943	0.02436	C	1.50556	-1.42447	-0.52644
H	-1.23344	0.89987	0.34377	H	1.70679	-1.97488	-1.45700
Si	-2.19136	-1.33526	-0.75589	C	1.59608	-2.36266	0.63847
C	1.20419	-1.15106	2.17066	C	0.82914	-2.16653	1.71374
H	-0.37357	-1.58208	3.70673	C	-0.09055	-0.98220	1.83196
C	1.23369	-0.15122	1.01529	C	-0.51390	-0.37357	0.49611
H	1.60219	-2.11118	1.81307	H	-1.76109	-0.93065	0.35274
H	1.88302	-0.80021	2.95759	C	-0.60559	1.08888	0.39865
H	0.93142	0.83382	1.40109	C	-0.99790	1.85877	1.51298
C	2.56979	-0.03998	0.32926	C	-1.21142	3.22939	1.40233
C	-1.81784	-3.17131	-0.92927	C	-1.04366	3.88319	0.18100
C	-1.78742	-0.49369	-2.42017	C	-0.66819	3.13342	-0.93404

C	-4.00391	-1.05111	-0.34711	C	-0.46113	1.76103	-0.83112
H	-0.75351	-3.32480	-1.13472	O	0.14471	-0.96289	-0.66291
H	-2.39427	-3.63254	-1.73830	H	3.80797	1.49481	-2.11336
H	-2.05428	-3.69570	0.00210	H	2.58292	0.46122	-2.86194
H	-0.73989	-0.64385	-2.72219	H	2.09052	1.83929	-1.85720
H	-2.02858	0.57895	-2.41341	H	3.65908	1.59194	1.21780
H	-2.38701	-0.93019	-3.22501	H	1.88582	1.58767	1.17716
H	-4.25983	-1.49022	0.62277	H	2.76603	0.29443	2.02554
H	-4.64939	-1.51261	-1.10167	H	5.33697	-0.37299	-0.46962
H	-4.23564	0.01793	-0.30461	H	4.56874	-1.65729	0.47229
C	3.38819	1.06985	0.54705	H	4.54235	-1.71595	-1.30013
C	3.01443	-1.05995	-0.51922	H	2.29931	-3.19010	0.58528
C	4.63942	1.15810	-0.06277	H	0.88000	-2.85061	2.55721
C	5.07747	0.13783	-0.90425	H	-0.98889	-1.28254	2.39404
C	4.26104	-0.97042	-1.13359	H	0.41661	-0.22974	2.45602
H	2.37162	-1.91869	-0.69502	H	-1.14577	1.37692	2.47550
H	4.59852	-1.76677	-1.79006	H	-1.51042	3.79330	2.28154
H	6.05029	0.20597	-1.38121	H	-1.20781	4.95249	0.09903
H	3.04236	1.86858	1.19941	H	-0.53639	3.62090	-1.89655
H	5.26825	2.02474	0.11691	H	-0.17452	1.19386	-1.71190
C	-1.07100	2.39993	-0.02786	Li	-1.48133	-1.54024	-1.24433
H	-0.64207	2.83401	0.88659	C	-3.03938	-1.74659	0.03244
C	-2.55879	2.73807	-0.09096	C	-3.83044	-1.02274	-1.05839
H	-2.72782	3.79558	-0.36136	H	-3.56069	-1.62368	0.98746
H	-3.03923	2.15507	-0.89750	H	-4.75394	-1.56673	-1.32430
C	-3.27766	2.44270	1.22622	H	-3.27282	-1.00363	-2.02861
H	-3.13865	1.39831	1.52629	C	-4.17293	0.42095	-0.68780
H	-2.87097	3.06806	2.02834	H	-4.79969	0.43281	0.20966
Li	-0.19163	0.83206	-1.12880	H	-3.27043	1.00098	-0.46562
C	-0.32765	3.00962	-1.23070	C	-2.89467	-3.23943	-0.27640
H	-0.63631	2.56608	-2.20008	H	-2.29823	-3.44981	-1.19094
H	0.76627	2.90030	-1.15454	H	-2.38809	-3.77283	0.53364
H	-0.51838	4.08595	-1.36668	H	-3.85656	-3.74422	-0.46848
H	-4.35283	2.63722	1.15784	H	-4.71844	0.92909	-1.48837
One imaginary frequency: -1250.42 cm^{-1}				One imaginary frequency: -1264.10 cm^{-1}			
Electronic Energy = -1075.237793				Electronic Energy = -1075.224132			
Zero-point corrected electronic energy=-1074.814983				Zero-point corrected electronic energy=-1074.801136			
Zero-point corrected Gibbs free energy=-1074.845003				Zero-point corrected Gibbs free energy=-1074.831359			

10. Energies and Cartesian coordinates of optimized geometries for stationary points of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism obtained at 195 K in the solvent at M062X/6-311++G(d,p) level of theory

1b-deprotonated Lithiated Intermediate				2a-deprotonated Lithiated Intermediate			
C	4.39445	-0.05874	0.37748	C	3.17974	-1.09302	-1.39728
Si	2.65891	-0.74670	0.12174	C	0.63014	-2.33854	-0.26610

C	2.07921	-1.59875	1.70806
C	2.69288	-2.07820	-1.21497
C	1.54263	0.63296	-0.34927
C	1.65559	2.01407	-0.11836
C	0.56949	2.87258	-0.13607
C	-0.83394	2.33337	0.08459
C	-0.76516	0.82183	0.30418
H	-0.36134	0.62452	1.30676
C	-2.08218	0.09343	0.14931
C	-3.29161	0.71371	0.47084
C	-4.49596	0.02362	0.36253
C	-4.50971	-1.29654	-0.07696
C	-3.30930	-1.92216	-0.40166
C	-2.10535	-1.23318	-0.28712
O	0.17336	0.26288	-0.63322
H	5.09958	-0.86825	0.58578
H	4.74472	0.47092	-0.51266
H	4.42374	0.63635	1.22064
H	2.69178	-2.47349	1.94718
H	2.11883	-0.90977	2.55613
H	1.04328	-1.93578	1.59998
H	3.28663	-2.94163	-0.90053
H	1.67872	-2.43026	-1.42685
H	3.11624	-1.69243	-2.14626
H	2.65818	2.41983	0.00527
H	0.72876	3.93557	-0.00199
H	-1.28042	2.79728	0.97325
H	-1.52476	2.54349	-0.74359
H	-3.29968	1.74383	0.80844
H	-5.42445	0.52162	0.61713
H	-5.44749	-1.83239	-0.16576
H	-3.30936	-2.95051	-0.74501
H	-1.17152	-1.71911	-0.54204
Li	0.79019	1.50097	-2.10334

Electronic Energy = -917.0983167
Zero-point corrected electronic energy= -916.805401
Zero-point corrected Gibbs free energy= -916.832326

C	2.77391	-1.37880	1.64871
C	1.24511	0.71903	0.03513
C	1.13828	1.64870	-1.00632
C	0.33328	2.77465	-0.92985
C	-0.80702	2.83937	0.07410
C	-0.86245	1.56678	0.92832
H	-1.25713	1.80215	1.91894
C	-1.68482	0.43018	0.36726
C	-2.33094	-0.43414	1.25398
C	-3.07087	-1.51631	0.78803
C	-3.17230	-1.74867	-0.58106
C	-2.53194	-0.89384	-1.47336
C	-1.79046	0.18658	-1.00339
O	0.49778	1.12591	1.19796
H	3.63572	-2.08691	-1.42394
H	3.97960	-0.35747	-1.27796
H	2.70207	-0.92268	-2.36605
H	1.06811	-3.33566	-0.15307
H	0.20103	-2.25924	-1.26843
H	-0.19308	-2.23910	0.44783
H	3.13839	-2.41004	1.66866
H	2.07231	-1.25628	2.47891
H	3.62302	-0.71255	1.82368
H	1.76087	1.48989	-1.88509
H	0.31485	3.47367	-1.75739
H	-1.77065	2.95420	-0.43924
H	-0.73106	3.70271	0.74576
H	-2.25465	-0.25271	2.32187
H	-3.56960	-2.17401	1.49077
H	-3.74866	-2.58974	-0.94903
H	-2.60600	-1.07154	-2.54040
H	-1.29362	0.85175	-1.70104
Si	1.92475	-0.98977	0.00777
Li	1.90060	2.55709	0.84791

Electronic Energy = -917.0994548
Zero-point corrected electronic energy= -916.806064
Zero-point corrected Gibbs free energy= -916.831097

B			
C	-1.02136	2.05477	0.46337
C	0.05125	2.76063	0.85954
H	-1.96202	2.25362	0.97661
O	-0.58882	0.95968	-1.60691
Si	-2.19508	-0.61688	-0.06334
C	1.52610	2.65412	0.56959
H	-0.15766	3.50929	1.62446
C	2.09324	1.65951	-0.41213
H	1.84371	3.66874	0.29636

C			
O	-2.35975	0.67951	-1.06939
C	-1.25920	0.59344	-0.22071
C	-1.47366	1.50567	0.98491
C	-0.87133	2.68490	0.84535
C	-0.06698	2.74916	-0.43088
C	0.01084	1.26947	-0.87828
H	-0.11212	1.16619	-1.95796
C	1.32441	0.62852	-0.48821
C	1.96932	0.91202	0.72147

H	1.95783	2.51239	1.58347
H	3.01879	2.00206	-0.87756
C	2.10751	0.27094	-0.07744
C	-3.91039	-0.24083	-0.73674
C	-1.41819	-2.05833	-0.96262
C	-2.28132	-0.84099	1.79591
H	-3.87432	-0.06139	-1.81393
H	-4.57995	-1.08634	-0.55595
H	-4.34394	0.63981	-0.25621
H	-1.45649	-1.89085	-2.04148
H	-0.37249	-2.17348	-0.66592
H	-1.94990	-2.98723	-0.74065
H	-2.74961	0.02613	2.26910
H	-2.88180	-1.72100	2.04272
H	-1.28857	-0.97276	2.23011
C	2.87256	-0.66715	-0.83678
C	1.37164	-0.28982	1.00590
C	2.89643	-2.01619	-0.54478
C	2.16390	-2.53926	0.53249
C	1.41544	-1.65238	1.29769
H	0.79356	0.35996	1.65370
H	0.84968	-2.02617	2.14688
H	3.46259	-0.29305	-1.67004
H	3.50121	-2.67899	-1.15664
C	-1.11404	0.93175	-0.49361
Li	0.97622	1.77171	-2.27553
H	2.18572	-3.59764	0.76138

Electronic Energy = -917.0867503
Zero-point corrected electronic energy= -916.797076
Zero-point corrected Gibbs free energy= -916.82265

C	3.15121	0.26825	1.07319
C	3.71899	-0.67688	0.22202
C	3.09918	-0.95845	-0.99198
C	1.92005	-0.30554	-1.34057
Si	-1.17496	-1.26431	0.25619
C	-2.86102	-1.68065	1.00526
C	-0.96024	-2.35070	-1.26993
C	0.11766	-1.75825	1.54408
H	-2.15015	1.24725	1.79508
H	-0.96920	3.52792	1.52213
H	0.92467	3.18854	-0.29046
H	-0.58516	3.36721	-1.17184
H	1.53422	1.63503	1.40279
H	3.62857	0.50063	2.01876
H	4.63762	-1.18125	0.49828
H	3.53685	-1.68078	-1.67217
H	1.44863	-0.52209	-2.29412
H	-2.87951	-2.72335	1.33650
H	-3.65571	-1.54710	0.26765
H	-3.08886	-1.05260	1.87121
H	-1.25995	-3.37837	-1.04212
H	0.07633	-2.37345	-1.61128
H	-1.58691	-1.98548	-2.08715
H	-0.10933	-2.75713	1.93071
H	0.11767	-1.06319	2.38922
H	1.12645	-1.77273	1.12407
Li	-4.07402	0.79443	-1.23841

Electronic Energy = -917.136539
Zero-point corrected electronic energy= -916.843325
Zero-point corrected Gibbs free energy= -916.868288

D

O	-1.51447	1.65465	-0.26785
C	-1.78670	0.36637	-0.21166
Si	-3.56269	-0.04206	0.30372
C	-3.91148	-1.89251	0.24075
C	-3.86787	0.58771	2.05401
C	-4.74982	0.85171	-0.85650
C	-0.90118	-0.62471	-0.50001
C	0.49370	-0.38165	-0.93098
C	1.23374	-1.40510	-1.74161
C	1.64580	-1.16752	-0.31000
H	1.34609	-1.92855	0.40227
C	2.92756	-0.49153	0.01025
C	3.47897	0.48440	-0.82966
C	4.67311	1.11703	-0.50409
C	5.34794	0.78840	0.66956
C	4.81271	-0.18114	1.51223

TS-B

C	1.06249	1.76001	-1.08648
C	0.07370	2.69501	-1.21576
C	1.17333	0.93760	0.07004
H	1.71512	1.55643	-1.93349
O	0.50687	1.35995	1.12562
Si	1.93077	-0.77670	0.07284
C	-1.09678	2.84309	-0.27222
H	-0.00101	3.25006	-2.14634
C	-1.40679	1.69405	0.64123
H	-1.00419	3.75278	0.33323
H	-1.98514	3.00614	-0.90157
H	-1.78928	1.97701	1.61808
C	-1.80522	0.39538	0.20972
C	3.67808	-0.72183	0.80731
C	0.90967	-1.92929	1.15385
C	2.09405	-1.47230	-1.67200

C	3.61592	-0.81209	1.18526
H	-4.94745	-2.09421	0.52819
H	-3.26027	-2.44412	0.92377
H	-3.75915	-2.28849	-0.76676
H	-4.91001	0.43618	2.34958
H	-3.64963	1.65655	2.12120
H	-3.23078	0.06694	2.77346
H	-5.78967	0.67038	-0.57007
H	-4.61760	0.51495	-1.88808
H	-4.57533	1.93024	-0.82720
H	-1.22284	-1.66041	-0.42449
H	0.73035	0.65669	-1.13729
H	0.71483	-2.33125	-1.95888
H	1.91668	-1.07083	-2.51401
H	2.97131	0.75577	-1.74951
H	5.08016	1.86877	-1.17101
H	6.27931	1.28110	0.92191
H	5.32760	-0.44866	2.42805
H	3.20653	-1.56628	1.84948
Li	-1.23036	3.30356	-0.70840

Electronic Energy = -917.1315736
Zero-point corrected electronic energy= -916.840756
Zero-point corrected Gibbs free energy= -916.869499

H	3.66105	-0.33260	1.82967
H	4.12764	-1.71943	0.83618
H	4.33022	-0.07403	0.21431
H	1.40692	-2.89798	1.26188
H	0.78109	-1.50429	2.15321
H	-0.08298	-2.08704	0.72529
H	2.69863	-0.81528	-2.30377
H	2.57707	-2.45396	-1.65525
H	1.10909	-1.57770	-2.13332
C	-2.52781	-0.44928	1.09701
C	-1.44499	-0.15149	-1.04548
C	-2.89682	-1.72951	0.74559
C	-2.55208	-2.24671	-0.51637
C	-1.83954	-1.44830	-1.39580
H	-0.91582	0.45359	-1.76605
H	-1.56934	-1.83455	-2.37365
H	-2.84063	-3.25388	-0.79346
H	-2.80692	-0.05849	2.07168
H	-3.45801	-2.33967	1.44518
Li	0.81097	1.96282	2.78989

One imaginary frequency: -364.18 cm^{-1}
Electronic Energy = -917.0645806
Zero-point corrected electronic energy= -916.774938
Zero-point corrected Gibbs free energy= -916.799757

TS-C

C	1.60770	1.86991	-0.78690
C	0.70710	2.83716	-0.59316
C	1.71486	0.74172	0.22637
H	2.36734	1.92885	-1.56368
O	2.46549	0.97134	1.21586
Si	1.65993	-1.12794	-0.19935
C	-0.22348	2.67834	0.59314
H	0.67747	3.73234	-1.20998
C	-0.34442	1.20805	0.95337
H	0.21191	3.24111	1.42593
H	-1.19186	3.14892	0.39253
H	0.00913	0.92801	1.93868
C	-1.53941	0.49450	0.55273
C	1.31146	-2.06654	1.38987
C	0.37948	-1.59959	-1.52447
C	3.34702	-1.58857	-0.88879
H	0.42111	-2.69229	1.29745
H	2.15692	-2.70881	1.64723
H	1.16089	-1.36386	2.21215
H	-0.66897	-1.47637	-1.22578
H	0.55603	-1.13497	-2.50122
H	0.50386	-2.67299	-1.69569

TS-D

C	-1.03403	-0.89309	-0.47386
C	0.21593	-1.13725	0.04038
C	-1.92000	0.15399	-0.00982
H	-1.37019	-1.48705	-1.31858
O	-1.43755	1.19898	0.48546
Si	-3.83964	0.01633	-0.15707
C	0.83347	-0.58443	1.27760
H	0.83055	-1.85355	-0.50271
C	1.69333	0.49641	0.65953
H	0.08619	-0.16278	1.94832
H	1.40230	-1.34987	1.81794
H	1.45262	1.51018	0.97669
C	3.04716	0.25923	0.26419
C	-4.43918	-0.55266	1.52741
C	-4.48836	1.72625	-0.55756
C	-4.28473	-1.22990	-1.48550
H	-4.12770	0.14876	2.30506
H	-5.53047	-0.61548	1.54192
H	-4.03775	-1.53864	1.77334
H	-4.13134	2.44609	0.18258
H	-4.15337	2.05617	-1.54381
H	-5.58115	1.73798	-0.54827

H	4.12845	-1.33025	-0.17020	H	-3.88213	-2.21891	-1.25294
H	3.40333	-2.66358	-1.08245	H	-5.37138	-1.32198	-1.56543
H	3.55659	-1.06346	-1.82441	H	-3.90163	-0.92420	-2.46241
C	-1.87876	-0.73943	1.17451	C	3.91168	1.34230	-0.05846
C	-2.38128	0.89914	-0.51675	C	3.62157	-1.03562	0.16523
C	-2.92264	-1.52120	0.72649	C	5.22363	1.14622	-0.45073
C	-3.70641	-1.12423	-0.36879	C	5.76244	-0.14161	-0.54897
C	-3.43123	0.09364	-0.97017	C	4.94032	-1.22159	-0.23212
H	-2.24056	1.87176	-0.98559	H	3.02175	-1.90900	0.39912
H	-4.04413	0.44221	-1.79457	H	5.33328	-2.23175	-0.29358
H	-4.52142	-1.74476	-0.71916	H	6.78872	-0.29388	-0.85908
H	-1.29101	-1.06281	2.02673	H	3.52218	2.35390	0.01568
H	-3.14215	-2.45497	1.23328	H	5.84151	2.00827	-0.68246
Li	-0.28529	0.66632	-1.38062	Li	0.18802	1.28523	-0.77336
One imaginary frequency: -168.50 cm^{-1} Electronic Energy = -917.0606671 Zero-point corrected electronic energy= -916.769861 Zero-point corrected Gibbs free energy= -916.794683				One imaginary frequency: -265.55 cm^{-1} Electronic Energy = -917.0760668 Zero-point corrected electronic energy= -916.787011 Zero-point corrected Gibbs free energy= -916.813852			

11. Energies and Cartesian coordinates of optimized geometries for stationary points of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism obtained at 195 K in the solvent at M062X/cc-pVTZ level of theory

1b-deprotonated Lithiated Intermediate				2a-deprotonated Lithiated Intermediate			
C	4.39865	-0.01630	0.35134	C	3.20436	-1.05646	-1.38920
Si	2.67595	-0.73819	0.11484	C	0.66101	-2.33821	-0.29188
C	2.14464	-1.62507	1.69679	C	2.76870	-1.36525	1.65089
C	2.71333	-2.05082	-1.23806	C	1.23600	0.72080	0.03587
C	1.52978	0.62627	-0.32194	C	1.11919	1.64763	-1.00184
C	1.63780	2.00342	-0.09295	C	0.31162	2.76663	-0.92417
C	0.55504	2.85989	-0.12330	C	-0.82216	2.82813	0.08204
C	-0.84813	2.32201	0.07816	C	-0.87136	1.55665	0.93161
C	-0.78101	0.81489	0.30535	H	-1.26758	1.78801	1.92043
H	-0.38828	0.62730	1.31212	C	-1.68894	0.42074	0.36970
C	-2.09544	0.08803	0.14769	C	-2.31599	-0.45555	1.25282
C	-3.30379	0.71571	0.44262	C	-3.04949	-1.53719	0.78663
C	-4.50577	0.02867	0.33675	C	-3.16401	-1.75727	-0.57991
C	-4.51893	-1.29688	-0.07401	C	-2.54379	-0.89002	-1.46896
C	-3.32012	-1.93026	-0.37328	C	-1.80946	0.19038	-0.99816
C	-2.11872	-1.24400	-0.26053	O	0.48764	1.11868	1.19918
O	0.16622	0.25089	-0.61647	H	3.66760	-2.04427	-1.42268
H	5.12359	-0.81126	0.53400	H	3.99441	-0.31634	-1.25480
H	4.71851	0.53433	-0.53472	H	2.73310	-0.87935	-2.35737
H	4.42504	0.66475	1.20312	H	1.10376	-3.32939	-0.16895
H	2.78359	-2.48413	1.91176	H	0.25125	-2.26452	-1.30046
H	2.17927	-0.94840	2.55204	H	-0.17380	-2.24267	0.40593

H	1.11874	-1.98765	1.59908
H	3.31997	-2.90817	-0.94022
H	1.70271	-2.41164	-1.44097
H	3.12013	-1.64928	-2.16740
H	2.63671	2.40881	0.04212
H	0.71293	3.92023	0.01500
H	-1.30837	2.78881	0.95558
H	-1.52777	2.52657	-0.75807
H	-3.31156	1.75045	0.75850
H	-5.43360	0.53324	0.57138
H	-5.45551	-1.83095	-0.16095
H	-3.31933	-2.96352	-0.69474
H	-1.18609	-1.73807	-0.49503
Li	0.79076	1.51095	-2.06211

Electronic Energy = -917.165407
Zero-point corrected electronic energy= -916.87203
Zero-point corrected Gibbs free energy= -916.898577

H	3.13843	-2.39204	1.67347
H	2.05559	-1.24846	2.46922
H	3.60892	-0.69461	1.83799
H	1.73776	1.49210	-1.88151
H	0.28570	3.46183	-1.75181
H	-1.78628	2.94228	-0.42605
H	-0.74685	3.68856	0.75402
H	-2.22851	-0.28313	2.31935
H	-3.53331	-2.20464	1.48738
H	-3.73543	-2.59865	-0.94863
H	-2.62939	-1.05743	-2.53468
H	-1.32913	0.86695	-1.69324
Si	1.93653	-0.97777	0.00280
Li	1.87571	2.55638	0.83569

Electronic Energy = -917.1657601
Zero-point corrected electronic energy= -916.87195
Zero-point corrected Gibbs free energy= -916.896886

B

C	-1.01875	2.04581	0.45692
C	0.04853	2.75179	0.85404
H	-1.95893	2.24350	0.96710
O	-0.58358	0.94615	-1.60672
Si	-2.20024	-0.61667	-0.06075
C	1.52103	2.64940	0.56877
H	-0.16249	3.49905	1.61634
C	2.09474	1.65855	-0.40704
H	1.83613	3.66326	0.29844
H	1.94623	2.51106	1.58390
H	3.01295	2.00465	-0.87852
C	2.11095	0.27334	-0.07694
C	-3.90724	-0.22470	-0.73991
C	-1.43446	-2.06635	-0.95272
C	-2.28634	-0.83694	1.79694
H	-3.86255	-0.04843	-1.81509
H	-4.58551	-1.06035	-0.55996
H	-4.32999	0.66087	-0.26400
H	-1.44794	-1.89170	-2.02875
H	-0.39933	-2.20229	-0.63539
H	-1.98794	-2.98335	-0.74614
H	-2.73737	0.03708	2.26889
H	-2.89840	-1.70563	2.04500
H	-1.29495	-0.98372	2.22429
C	2.87719	-0.66036	-0.83388
C	1.37673	-0.28958	1.00168
C	2.90280	-2.00601	-0.54471
C	2.17078	-2.53124	0.52724
C	1.42190	-1.64901	1.29046

C

O	2.37052	0.66218	1.03622
C	1.26971	0.57766	0.19446
C	1.49089	1.46664	-1.02256
C	0.89891	2.64894	-0.90579
C	0.09799	2.74505	0.36651
C	0.00989	1.27843	0.84470
H	0.14010	1.19643	1.92320
C	-1.30991	0.64343	0.48196
C	-1.96792	0.91594	-0.71875
C	-3.15534	0.27735	-1.04617
C	-3.71708	-0.65003	-0.17765
C	-3.08469	-0.91974	1.02851
C	-1.89920	-0.27337	1.35155
Si	1.16744	-1.28238	-0.26253
C	2.81834	-1.71268	-1.07175
C	0.98710	-2.34616	1.28216
C	-0.16473	-1.78550	-1.50342
H	2.16371	1.18673	-1.82556
H	1.00106	3.47566	-1.59832
H	-0.88905	3.18637	0.21787
H	0.61748	3.37605	1.09236
H	-1.53768	1.62626	-1.41322
H	-3.64258	0.50080	-1.98644
H	-4.64127	-1.14986	-0.43462
H	-3.51759	-1.62851	1.72247
H	-1.41759	-0.48043	2.29978
H	2.86106	-2.78232	-1.28733
H	3.65412	-1.45980	-0.42009
H	2.94877	-1.18002	-2.01545

H	0.79845	0.35729	1.64880	H	1.24239	-3.38302	1.05326
H	0.85639	-2.02344	2.13696	H	-0.03314	-2.33086	1.66423
H	3.46747	-0.28417	-1.66344	H	1.65628	-1.99465	2.06785
H	3.50899	-2.66530	-1.15527	H	0.04428	-2.79054	-1.87764
C	-1.11031	0.92333	-0.49453	H	-0.17810	-1.10546	-2.35783
Li	0.97040	1.76516	-2.25701	H	-1.16057	-1.78273	-1.05864
H	2.19428	-3.58780	0.75413	Li	3.91206	0.99333	1.66573
Electronic Energy = -917.1517087 Zero-point corrected electronic energy= -916.861844 Zero-point corrected Gibbs free energy= -916.887416				Electronic Energy = -917.2013436 Zero-point corrected electronic energy= -916.907987 Zero-point corrected Gibbs free energy= -916.933004			
D				TS-B			
C	1.00707	1.12025	-0.09394	C	1.04916	1.75662	-1.08168
C	-0.43538	1.29336	-0.38330	C	0.06204	2.68713	-1.21157
C	1.64378	-0.05884	-0.30611	C	1.16425	0.93698	0.07102
H	1.56218	1.97018	0.28563	H	1.70105	1.55446	-1.92693
O	1.04657	-1.14091	-0.75589	O	0.49640	1.35559	1.12689
Si	3.49403	-0.24904	0.04407	Si	1.93749	-0.76705	0.07133
C	-1.20620	2.43656	0.18069	C	-1.10692	2.83275	-0.27149
H	-0.76391	0.94231	-1.35732	H	-0.01432	3.23949	-2.14088
C	-1.48363	1.05022	0.69969	C	-1.41471	1.68577	0.63898
H	-1.97580	2.90177	-0.41956	H	-1.02111	3.74212	0.33171
H	-0.67653	3.10804	0.84265	H	-1.99261	2.99153	-0.90213
H	-1.07851	0.82130	1.67633	H	-1.79510	1.96629	1.61474
C	-2.73983	0.34218	0.37051	C	-1.80654	0.38871	0.20964
C	4.25339	1.34499	0.69658	C	3.67722	-0.70001	0.81783
C	3.73125	-1.61884	1.31573	C	0.91996	-1.93322	1.13908
C	4.38078	-0.75342	-1.53898	C	2.11674	-1.45328	-1.67383
H	3.77039	1.66119	1.62226	H	3.64818	-0.30958	1.83716
H	5.31617	1.20361	0.90096	H	4.13245	-1.69236	0.85177
H	4.15375	2.15181	-0.03087	H	4.32706	-0.04941	0.22958
H	3.26298	-1.35518	2.26519	H	1.42011	-2.89841	1.24104
H	3.28006	-2.54648	0.96106	H	0.78665	-1.51632	2.13888
H	4.79082	-1.80539	1.49886	H	-0.06872	-2.09042	0.70566
H	4.28927	0.02186	-2.30098	H	2.71375	-0.78674	-2.29881
H	5.44257	-0.92378	-1.35211	H	2.61108	-2.42676	-1.65881
H	3.95586	-1.67432	-1.94007	H	1.13636	-1.56838	-2.13772
C	-3.25736	-0.60681	1.25497	C	-2.52298	-0.45717	1.09500
C	-3.42886	0.56716	-0.82466	C	-1.44954	-0.15475	-1.04375
C	-4.41875	-1.30710	0.95883	C	-2.88637	-1.73533	0.74521
C	-5.09158	-1.07421	-0.23311	C	-2.54390	-2.24916	-0.51463
C	-4.58937	-0.13202	-1.12244	C	-1.83872	-1.44949	-1.39291
H	-3.05748	1.29868	-1.53187	H	-0.92580	0.45270	-1.76326
H	-5.10583	0.06227	-2.05329	H	-1.57048	-1.83300	-2.37009
H	-5.99797	-1.61627	-0.46543	H	-2.82770	-3.25573	-0.79051
H	-2.74193	-0.79159	2.18964	H	-2.80102	-0.06786	2.06844
H	-4.80100	-2.03353	1.66402	H	-3.44279	-2.34659	1.44443
Li	-0.36865	-2.13451	-0.95721	Li	0.78955	1.95189	2.78351

Electronic Energy = -917.1991858 Zero-point corrected electronic energy= -916.90719 Zero-point corrected Gibbs free energy= -916.934545	One imaginary frequency: -371.08 cm^{-1} Electronic Energy = -917.1289071 Zero-point corrected electronic energy= -916.839271 Zero-point corrected Gibbs free energy= -916.86437
TS-C C 1.58427 1.87952 -0.77499 C 0.68080 2.84080 -0.59522 C 1.67058 0.74828 0.23238 H 2.35161 1.93653 -1.54110 O 2.42143 0.96243 1.22715 Si 1.67799 -1.11985 -0.20102 C -0.25588 2.67748 0.58132 H 0.65337 3.73440 -1.21012 C -0.36067 1.20922 0.94441 H 0.16389 3.24826 1.41370 H -1.22695 3.13287 0.37173 H -0.01634 0.93924 1.93334 C -1.54932 0.48646 0.54426 C 1.33262 -2.07013 1.37750 C 0.42802 -1.63761 -1.53746 C 3.39287 -1.50430 -0.85955 H 0.36781 -2.57438 1.33579 H 2.10389 -2.82118 1.55026 H 1.33488 -1.37844 2.22006 H -0.62185 -1.54284 -1.23874 H 0.58877 -1.16351 -2.51027 H 0.58664 -2.70456 -1.70571 H 4.14183 -1.18551 -0.13407 H 3.51298 -2.57541 -1.03018 H 3.58571 -0.98565 -1.79972 C -1.88762 -0.73827 1.17344 C -2.38151 0.87868 -0.53057 C -2.92665 -1.52342 0.72903 C -3.70278 -1.13777 -0.37035 C -3.42527 0.07064 -0.98157 H -2.23405 1.84285 -1.00911 H -4.03116 0.40919 -1.81249 H -4.51415 -1.76059 -0.71863 H -1.30465 -1.05048 2.03072 H -3.14797 -2.45069 1.24232 Li -0.25145 0.61697 -1.32881 One imaginary frequency: -189.85 cm^{-1} Electronic Energy = -917.1244571 Zero-point corrected electronic energy= -916.833035 Zero-point corrected Gibbs free energy= -	TS-D C -1.03501 -0.88912 -0.45636 C 0.20793 -1.12649 0.06043 C -1.92586 0.15830 -0.00926 H -1.37405 -1.50004 -1.28485 O -1.45354 1.21248 0.47258 Si -3.84361 0.00761 -0.15921 C 0.83832 -0.53923 1.27273 H 0.81615 -1.85841 -0.46453 C 1.70580 0.52554 0.64049 H 0.09736 -0.10193 1.93705 H 1.40409 -1.29429 1.82715 H 1.48346 1.54223 0.95491 C 3.05394 0.26951 0.25155 C -4.44350 -0.44629 1.55713 C -4.49219 1.68505 -0.67444 C -4.27616 -1.32784 -1.39904 H -4.13093 0.30560 2.28240 H -5.53252 -0.50745 1.57520 H -4.04218 -1.41119 1.86801 H -4.13026 2.45072 0.01200 H -4.16328 1.94352 -1.68123 H -5.58260 1.69690 -0.65856 H -3.87937 -2.29420 -1.08519 H -5.35954 -1.42257 -1.48722 H -3.87692 -1.09758 -2.38753 C 3.93118 1.33542 -0.07949 C 3.61401 -1.02910 0.16987 C 5.23938 1.12082 -0.46035 C 5.76390 -0.17038 -0.53932 C 4.92948 -1.23385 -0.21629 H 3.00429 -1.89143 0.41002 H 5.31041 -2.24727 -0.26335 H 6.78844 -0.33750 -0.84032 H 3.55298 2.35026 -0.02007 H 5.86651 1.97198 -0.69805 Li 0.17316 1.30074 -0.75114 One imaginary frequency: -236.94 cm^{-1} Electronic Energy = -917.1425023 Zero-point corrected electronic energy= -916.853495 Zero-point corrected Gibbs free energy= -

916.857731	916.880598

12. Energies and Cartesian Coordinates for optimized geometries of Intermediates B, C, D, and products 3a and 4a of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism in gas phase at 195 K

B			
C	-0.94634	2.10106	0.15532
C	0.10413	2.83235	0.57983
H	-1.92118	2.39954	0.54773
O	-0.42926	0.63549	-1.67862
Si	-2.27527	-0.52553	-0.03082
C	1.60085	2.70476	0.47136
H	-0.17920	3.67035	1.22154
C	2.25555	1.64310	-0.36395
H	1.94626	3.69182	0.13390
H	1.93054	2.66516	1.53211
H	3.16514	1.96287	-0.87502
C	2.22997	0.27432	0.02044
C	-3.96076	-0.03987	-0.72056
C	-1.66062	-2.12358	-0.78151
C	-2.33936	-0.54531	1.84639
H	-3.93280	0.03196	-1.81197
H	-4.70918	-0.79271	-0.45083
H	-4.29774	0.92250	-0.32243
H	-1.69859	-2.06389	-1.87332
H	-0.62319	-2.31469	-0.48678
H	-2.27505	-2.97126	-0.46170
H	-2.73899	0.39598	2.23700
H	-2.98784	-1.35558	2.19623
H	-1.34518	-0.69563	2.27549
C	2.90962	-0.71699	-0.76141
C	1.41738	-0.24369	1.07900
C	2.80431	-2.07803	-0.49417
C	2.01443	-2.54771	0.55594
C	1.33711	-1.60469	1.33799
H	0.88548	0.45229	1.72383
H	0.73068	-1.94571	2.17508
H	3.59042	-0.38129	-1.54720
H	3.36062	-2.78068	-1.10989
C	-1.03966	0.84985	-0.62447
Li	1.36407	0.65253	-1.93696
H	1.93574	-3.60837	0.76636
Electronic Energy = -916.901238887 Zero-point corrected electronic energy=-916.609583 Zero-point corrected Gibbs free energy=-916.635436			

C			
O	-2.33015	0.73739	-1.07278
C	-1.21722	0.65599	-0.22874
C	-1.40267	1.60790	0.94881
C	-0.77351	2.76907	0.76015
C	0.01887	2.76620	-0.52543
C	0.05642	1.26999	-0.91746
H	-0.07762	1.12852	-1.99411
C	1.34458	0.59373	-0.49809
C	1.97959	0.87128	0.72061
C	3.12904	0.18366	1.10396
C	3.67140	-0.80081	0.27824
C	3.06048	-1.07815	-0.94310
C	1.91484	-0.38115	-1.32419
Si	-1.18822	-1.19471	0.26026
C	-3.00148	-1.52435	0.81758
C	-0.91257	-2.31372	-1.23365
C	-0.05661	-1.71705	1.67630
H	-2.07617	1.39506	1.77810
H	-0.84504	3.63900	1.40793
H	1.02446	3.18726	-0.41308
H	-0.50000	3.36320	-1.28545
H	1.55983	1.62278	1.38353
H	3.59967	0.41257	2.05583
H	4.56457	-1.33934	0.57980
H	3.47931	-1.83102	-1.60470
H	1.44796	-0.59494	-2.28309
H	-3.05280	-2.36567	1.51607
H	-3.63738	-1.82880	-0.03037
H	-3.44947	-0.66469	1.33498
H	-1.42453	-3.27318	-1.09762
H	0.14975	-2.52027	-1.38672
H	-1.30782	-1.83470	-2.13594
H	-0.33835	-2.70436	2.05952
H	-0.10146	-1.00148	2.50467
H	0.98364	-1.76592	1.33663
Li	-3.86308	0.12911	-0.86577
Electronic Energy = -916.933724093 Zero-point corrected electronic energy=-916.638997 Zero-point corrected Gibbs free energy=-916.664021			

D

O	-1.95976	-0.77157	-1.62681
C	-1.97151	-0.24013	-0.42248
Si	-3.67652	0.36709	0.16305
C	-4.84140	-1.11440	0.14233
C	-3.58861	1.10134	1.89778
C	-4.26408	1.64945	-1.07918
C	-0.83966	-0.19229	0.36410
C	0.51445	-0.51068	-0.19420
C	1.18255	-1.90300	-0.02690
C	1.69336	-0.68418	0.69810
H	1.46136	-0.66282	1.76209
C	3.02895	-0.11135	0.33465
C	3.13826	1.20309	-0.12557
C	4.38478	1.74370	-0.43677
C	5.53712	0.97420	-0.28924
C	5.43720	-0.33861	0.17047
C	4.19001	-0.87657	0.47832
H	-5.87259	-0.81737	0.35963
H	-4.54226	-1.86177	0.88520
H	-4.82108	-1.58366	-0.84636
H	-4.57250	1.46267	2.21530
H	-3.25507	0.35649	2.62807
H	-2.89395	1.94677	1.93342
H	-3.63671	2.54557	-1.04963
H	-4.20501	1.22879	-2.08754
H	-5.29936	1.94867	-0.88540
H	-0.89118	0.20129	1.37497
H	0.73155	-0.06421	-1.16583
H	1.80406	-2.28592	-0.83253
H	0.68970	-2.65382	0.59216
H	2.23783	1.80136	-0.24032
H	4.45507	2.76568	-0.79632
H	6.50821	1.39374	-0.53304
H	6.33111	-0.94445	0.28436
H	4.11005	-1.90183	0.83190
Li	-0.93271	-2.01514	-0.92228

Electronic Energy = -916.931850227
Zero-point corrected electronic energy=-916.638634
Zero-point corrected Gibbs free energy=-916.666182

3a

O	0.99735	-0.70596	-1.22751
C	1.63198	0.06350	-0.52739
C	1.01631	1.37647	-0.05714
C	-0.46522	1.47674	-0.31177
H	-0.76211	1.28363	-1.33950
C	-1.42229	0.95937	0.73297
H	-0.95868	0.60190	1.65025
C	-2.65317	0.21413	0.35259
C	-3.40103	0.54043	-0.78541
C	-4.54583	-0.17901	-1.11684
C	-4.96803	-1.24003	-0.31658
C	-4.23233	-1.57361	0.81821
C	-3.08686	-0.85189	1.14666
C	-1.29371	2.44424	0.47361
Si	3.42987	-0.41445	0.01688
C	4.11917	-1.55512	-1.29823
C	4.45743	1.15063	0.22064
C	3.25951	-1.29793	1.67073
H	1.56587	2.18658	-0.56220
H	1.23761	1.50197	1.01386
H	-3.08865	1.36240	-1.42520
H	-5.10957	0.08936	-2.00522
H	-5.85984	-1.80104	-0.57698
H	-4.54766	-2.39915	1.44911
H	-2.51613	-1.12016	2.03195
H	-0.79819	3.04431	1.23125
H	-2.12889	2.93393	-0.01737
H	4.27890	-1.02165	-2.23982
H	3.41055	-2.36612	-1.48981
H	5.07287	-1.99101	-0.98467
H	4.53913	1.70091	-0.72207
H	5.47197	0.90485	0.55161
H	4.01907	1.82097	0.96735
H	2.61821	-2.17921	1.57391
H	2.82472	-0.64176	2.43165
H	4.23835	-1.62832	2.03336

Electronic Energy = -909.967653391
Zero-point corrected electronic energy=-909.663967
Zero-point corrected Gibbs free energy=-909.691515

4a

O	-2.36046	0.70379	-1.20707
C	-1.26871	0.62732	-0.26118
Si	-1.32241	-1.24089	0.21638
C	-3.04399	-1.50205	0.93951
C	-1.14421	-2.27923	-1.34069
C	-0.05582	-1.73819	1.51648

C	-1.55303	1.57527	0.88613
C	-0.91032	2.73749	0.73964
C	-0.02528	2.74369	-0.48338
C	0.01986	1.24999	-0.89939
H	-0.07224	1.12771	-1.98305
C	1.30342	0.57500	-0.46022
C	1.89874	0.83903	0.77933
C	3.05546	0.17078	1.17314
C	3.64195	-0.77586	0.33372
C	3.06816	-1.03798	-0.90869
C	1.91326	-0.36228	-1.29942
H	-2.67501	1.61702	-1.24229
H	-3.23086	-2.57037	1.09319
H	-3.80801	-1.11235	0.26099
H	-3.15657	-1.00671	1.90979
H	-1.43552	-3.31505	-1.13568
H	-0.11489	-2.28877	-1.70893
H	-1.79592	-1.88848	-2.12795
H	-0.36020	-2.69291	1.96079
H	0.00224	-0.99819	2.32201
H	0.94757	-1.85949	1.09737
H	-2.27571	1.35102	1.66593
H	-1.02061	3.59858	1.39293
H	0.97552	3.14000	-0.28331
H	-0.45963	3.37788	-1.26739
H	1.44444	1.56272	1.45134
H	3.49718	0.38462	2.14191
H	3.52189	-1.76256	-1.57822
H	1.47503	-0.56171	-2.27454
H	4.54180	-1.29866	0.64247

Electronic Energy = -909.983156394
Zero-point corrected electronic energy=-909.677991
Zero-point corrected Gibbs free energy=-909.702592

13. Energies and Cartesian Coordinates for optimized geometries of transition states TS-B, TS-B' TS-C and TS- D of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism in gas phase at 195 K

TS-B				TS-B'			
C	-1.00386	1.85681	0.88091	C	-0.86391	1.76803	0.99865
C	-0.01472	2.78916	0.93420	C	0.10211	2.76724	0.99320
C	-1.07498	0.88114	-0.16007	H	-1.44378	1.59558	1.90493

H	-1.70412	1.78075	1.71170
O	-0.34149	1.11717	-1.25282
Si	-2.18011	-0.62555	-0.07975
C	1.11684	2.87745	-0.05196
H	0.03055	3.46511	1.78357
C	1.46078	1.62019	-0.80810
H	0.92279	3.66518	-0.79014
H	2.02342	3.18804	0.48942
H	1.80198	1.79387	-1.82645
C	1.98716	0.42739	-0.21802
C	-3.78652	-0.37642	-1.03368
C	-1.29876	-2.10373	-0.93309
C	-2.57816	-1.11090	1.69368
H	-3.57700	-0.13059	-2.07953
H	-4.41634	-1.27251	-1.00632
H	-4.35600	0.45539	-0.60688
H	-1.02278	-1.91339	-1.98152
H	-0.42841	-2.49138	-0.38126
H	-2.01152	-2.93278	-0.97978
H	-3.09259	-0.29616	2.21368
H	-3.23582	-1.98642	1.71927
H	-1.66605	-1.34378	2.25188
C	2.75824	-0.47492	-1.02073
C	1.53542	-0.05938	1.04324
C	3.08916	-1.74004	-0.57865
C	2.67338	-2.18569	0.69626
C	1.92063	-1.33731	1.49028
H	0.96425	0.59166	1.69153
H	1.59435	-1.66658	2.47323
H	2.94230	-3.17748	1.04348
H	3.09805	-0.13659	-1.99742
H	3.68720	-2.38960	-1.21103
Li	0.33047	-0.58834	-0.99473

One imaginary frequency: -385.24 cm^{-1}
Electronic Energy = -916.878212435
Zero-point corrected electronic energy=-916.585115
Zero-point corrected Gibbs free energy=-916.609894

O	-0.59451	1.32657	-1.25940
Si	-1.99287	-0.74733	-0.08434
C	1.37832	2.76311	0.10937
H	0.20937	3.35579	1.90073
C	1.69278	1.59613	-0.74415
H	1.48350	3.69610	-0.47313
H	2.16421	2.84565	0.87719
H	2.00974	1.79406	-1.76359
C	1.86400	0.27233	-0.27380
C	-3.70931	-0.48487	-0.83347
C	-1.02964	-1.95328	-1.14343
C	-2.18213	-1.33758	1.69393
H	-3.62318	-0.10258	-1.85596
H	-4.26981	-1.42539	-0.87089
H	-4.29457	0.23345	-0.24970
H	-0.74236	-1.46483	-2.08021
H	-0.11338	-2.26980	-0.63648
H	-1.62631	-2.84062	-1.37989
H	-2.75470	-0.62302	2.29521
H	-2.70908	-2.29703	1.72992
H	-1.19962	-1.46941	2.15799
C	2.39256	-0.71759	-1.15455
C	1.52620	-0.15121	1.03780
C	2.62063	-2.01054	-0.74017
C	2.31097	-2.40252	0.57751
C	1.77051	-1.46907	1.44798
H	1.15215	0.56141	1.76150
H	1.52985	-1.75642	2.46835
H	2.49167	-3.42190	0.90338
H	2.63379	-0.42510	-2.17375
H	3.03687	-2.73328	-1.43600
C	-1.08891	0.91897	-0.12878
Li	-0.66110	3.08084	-0.95475

One imaginary frequency: -181.93 cm^{-1}
Electronic Energy = -916.871234585
Zero-point corrected electronic energy=-916.579941
Zero-point corrected Gibbs free energy=-916.604749

TS-C

C	1.50106	1.83961	-0.81222
C	0.62850	2.84304	-0.65139
C	1.52666	0.74748	0.26978
H	2.28211	1.84614	-1.57152
O	2.35358	0.93503	1.21778
Si	1.64761	-1.13567	-0.17978
C	-0.26765	2.73812	0.56526
H	0.61569	3.72614	-1.28845

TS-D

C	1.00756	0.87358	-0.37210
C	-0.23814	1.05115	0.18125
C	1.95376	-0.17098	-0.01712
H	1.31992	1.56135	-1.15536
O	1.53292	-1.28984	0.37451
Si	3.86728	0.03823	-0.17542
C	-0.86911	0.36303	1.35125
H	-0.86056	1.80816	-0.29692

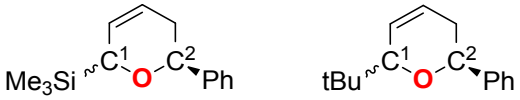
C	-0.33662	1.27372	0.97420	C	-1.74351	-0.66457	0.64284
H	0.18782	3.33815	1.36205	H	-0.11472	-0.12622	1.97225
H	-1.25734	3.17372	0.37789	H	-1.42367	1.07899	1.97655
H	-0.04364	1.05606	1.99754	H	-1.65472	-1.66683	1.07679
C	-1.53011	0.52839	0.56435	C	-3.09425	-0.31452	0.24160
C	1.35632	-2.13894	1.37343	C	4.52888	-0.10475	1.57448
C	0.39768	-1.68348	-1.54293	C	4.47795	-1.37960	-1.24324
C	3.37504	-1.38332	-0.87086	C	4.25650	1.71051	-0.93764
H	0.30572	-2.41947	1.48608	H	4.20694	-1.05033	2.02087
H	1.95680	-3.05383	1.36752	H	5.62319	-0.07892	1.57656
H	1.66090	-1.53106	2.23121	H	4.16829	0.71216	2.20640
H	-0.65814	-1.68074	-1.23173	H	4.11858	-2.33115	-0.84003
H	0.49635	-1.13529	-2.49327	H	4.12382	-1.28766	-2.27462
H	0.62589	-2.72472	-1.79421	H	5.57194	-1.40888	-1.26417
H	4.10117	-1.01038	-0.14294	H	3.81940	2.52347	-0.34922
H	3.57951	-2.44150	-1.06366	H	5.33869	1.87152	-0.97740
H	3.51793	-0.83291	-1.80658	H	3.87334	1.78580	-1.96038
C	-1.90006	-0.65976	1.24363	C	-4.00307	-1.32328	-0.16065
C	-2.27611	0.84619	-0.60037	C	-3.58671	1.00921	0.22132
C	-2.90957	-1.48274	0.77536	C	-5.29779	-1.03044	-0.56014
C	-3.60798	-1.16864	-0.40023	C	-5.75783	0.29060	-0.58513
C	-3.29049	0.00431	-1.07281	C	-4.88671	1.30125	-0.18677
H	-2.08901	1.78476	-1.12393	H	-2.94791	1.83071	0.53585
H	-3.84002	0.28498	-1.96689	H	-5.22167	2.33542	-0.18584
H	-4.39402	-1.82018	-0.76596	H	-6.76957	0.52101	-0.90188
H	-1.37104	-0.91360	2.15823	H	-3.66672	-2.35857	-0.15088
H	-3.16431	-2.38202	1.32906	H	-5.95967	-1.84037	-0.85572
Li	-0.13587	0.44368	-1.05901	Li	-0.14517	-1.25446	-0.53093
One imaginary frequency: -210.27 cm^{-1} Electronic Energy = -916.887822232 Zero-point corrected electronic energy=-916.597049 Zero-point corrected Gibbs free energy=-916.624006				One imaginary frequency: -246.70 cm^{-1} Electronic Energy = -916.877358731 Zero-point corrected electronic energy=-916.584762 Zero-point corrected Gibbs free energy=-916.609281			
[1,2]-Wittig concerted transition state (298 K)							
C	1.42307	-2.00923	1.48918				
Si	1.66292	-1.14250	-0.16615				
C	1.14422	0.63926	-0.00836				
C	0.91742	1.50645	-1.11366				
C	0.36628	2.75972	-0.88243				
C	-0.41447	2.83869	0.41997				
C	-0.48630	1.43827	1.02266				
H	-0.45309	1.40533	2.10690				
C	-1.47689	0.46808	0.49914				
C	-1.79609	-0.65672	1.27571				
C	-2.71604	-1.59728	0.82434				
C	-3.35241	-1.41469	-0.40411				
C	-3.07289	-0.27837	-1.16620				
C	-2.15114	0.66149	-0.71974				

O	1.45776	1.28664	1.26973
C	3.50201	-1.25234	-0.62359
C	0.63333	-1.95993	-1.51753
H	1.61313	-1.29343	2.29584
H	2.11478	-2.85065	1.59920
H	0.40460	-2.39301	1.59757
H	1.12423	1.16066	-2.12893
H	0.21096	3.49402	-1.66317
H	-1.43963	3.20053	0.23484
H	0.02400	3.49816	1.17771
H	-1.29777	-0.79500	2.23229
H	-2.94423	-2.46724	1.43263
H	-3.58305	-0.12186	-2.11175
H	-1.93736	1.54000	-1.31943
H	4.11897	-0.75095	0.13136
H	3.69599	-0.78204	-1.59410
H	3.83823	-2.29375	-0.68282
H	-0.43254	-1.89365	-1.26821
H	0.89390	-3.01794	-1.63014
H	0.78116	-1.47375	-2.48806
Li	2.42588	2.27349	0.14436
H	-4.07345	-2.14449	-0.75885

One imaginary frequency: -1160.07 cm^{-1}
Electronic Energy = -916.795047061
Zero-point corrected electronic energy= -916.503707
Zero-point corrected Gibbs free energy= -916.549926

14. Energies and Cartesian coordinates of optimized geometries for stationary points of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism obtained at 195 K in Tetrahydrofuran solvent

Numbering system followed for the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism



Reactants							
Silicon analogues				Carbon Analogues			
1a				1aC			
C	-2.68157	-2.12526	-0.89080	C	-2.93078	-1.12588	1.61094
Si	-2.63082	-0.56222	0.15177	C	-2.37766	-2.00687	-0.65476
C	-3.63159	0.81364	-0.64496	C	-3.53468	0.20654	-0.42817
C	-3.24889	-0.91220	1.89517	C	-1.10988	-0.05322	0.24986
C	-0.80585	0.00712	0.26845	H	-0.42023	-0.76883	0.73702

H	-0.22637	-0.79612	0.76285	C	-1.08466	1.23560	1.03036
C	-0.66265	1.27239	1.05857	C	-0.48585	2.33679	0.57232
C	-0.05228	2.35774	0.57343	C	0.22526	2.35592	-0.75425
C	0.60871	2.33787	-0.78021	C	0.50979	0.92951	-1.21780
C	0.85267	0.89767	-1.22393	H	0.71326	0.93035	-2.29397
H	1.05276	0.87703	-2.30066	C	1.67553	0.23006	-0.52660
C	1.99402	0.17091	-0.52227	C	1.98100	-1.07539	-0.93273
C	2.22450	-1.16489	-0.87538	C	3.02341	-1.78328	-0.34124
C	3.24624	-1.89756	-0.27794	C	3.78060	-1.19241	0.67278
C	4.05813	-1.30094	0.68898	C	3.48317	0.10357	1.08604
C	3.83602	0.02589	1.04920	C	2.43458	0.80944	0.49074
C	2.80723	0.75608	0.44905	O	-0.68080	0.15048	-1.09246
O	-0.36383	0.15561	-1.08312	H	-3.85134	-1.71687	1.56340
H	-3.70309	-2.51225	-0.96436	H	-3.13543	-0.25318	2.23803
H	-2.05211	-2.90559	-0.45038	H	-2.16546	-1.73508	2.10584
H	-2.31659	-1.92376	-1.90230	H	-3.33000	-2.54786	-0.65330
H	-4.67342	0.50746	-0.78494	H	-1.60674	-2.67342	-0.24963
H	-3.21529	1.07012	-1.62426	H	-2.11519	-1.76906	-1.68829
H	-3.62075	1.71479	-0.02341	H	-4.50581	-0.29616	-0.49417
H	-4.26706	-1.31377	1.86063	H	-3.23110	0.50611	-1.43548
H	-3.26943	-0.00320	2.50477	H	-3.66079	1.11154	0.17592
H	-2.61423	-1.64847	2.39931	H	-1.55623	1.23681	2.00971
H	-1.08897	1.27786	2.06052	H	-0.49734	3.24959	1.16369
H	-0.00298	3.26981	1.16334	H	1.15060	2.93864	-0.69608
H	1.54739	2.90204	-0.76568	H	-0.40049	2.85006	-1.50733
H	-0.03041	2.82593	-1.52601	H	1.38457	-1.53633	-1.71694
H	1.58580	-1.62844	-1.62362	H	3.24723	-2.79364	-0.67016
H	3.41124	-2.93158	-0.56562	H	4.59528	-1.73998	1.13661
H	4.85712	-1.86737	1.15754	H	4.06272	0.56974	1.87711
H	4.45954	0.49659	1.80335	H	2.21090	1.81358	0.83736
H	2.64086	1.78438	0.75489	C	-2.49683	-0.73369	0.19258
Electronic Energy = -909.982919075 Zero-point corrected electronic energy=-909.677885 Zero-point corrected Gibbs free energy=-909.704399				Electronic Energy = -658.5940971 Zero-point corrected electronic energy=-658.276684 Zero-point corrected Gibbs free energy=-658.300594			
1b				1bC			
C	2.10461	-0.91511	1.90125	C	-2.63780	0.16055	1.23060
Si	2.58008	-0.78619	0.08330	C	-3.96291	-0.26382	1.13966
C	2.27706	-2.42678	-0.78152	C	-4.45466	-0.76161	-0.06696
C	4.38847	-0.28013	-0.06322	C	-3.61454	-0.82988	-1.17888
C	1.55289	0.54808	-0.85384	C	-2.29134	-0.40017	-1.08767
H	1.90809	0.48740	-1.89423	C	-1.79308	0.09795	0.11942
C	1.77813	1.94505	-0.36514	H	-2.25418	0.54046	2.17502
C	0.79566	2.70951	0.12101	H	-4.60738	-0.21375	2.01203
C	-0.61213	2.18734	0.23038	H	-5.48424	-1.09829	-0.13904
C	-0.59795	0.65626	0.18869	H	-3.99069	-1.22003	-2.11990
H	-0.13158	0.29597	1.11786	H	-1.63303	-0.45680	-1.94891
C	-1.98910	0.08040	0.08908	C	-0.38133	0.62400	0.22210

C	-2.58633	-0.15183	-1.15281	H	-0.03057	0.49457	1.25521
C	-3.89246	-0.63479	-1.22594	O	0.43568	-0.12908	-0.66758
C	-4.61589	-0.88566	-0.05960	C	1.83011	0.17809	-0.68745
C	-4.02473	-0.65406	1.18236	C	2.40022	-2.23794	-0.41968
C	-2.71678	-0.17633	1.25390	H	2.75686	-2.30413	-1.45438
O	0.16134	0.20819	-0.92682	H	2.93512	-2.98967	0.17072
H	2.84773	-1.52356	2.42849	H	1.33423	-2.48062	-0.40680
H	2.07472	0.06971	2.37935	C	2.24000	-0.81603	1.63024
H	1.12919	-1.39449	2.03095	H	1.21785	-1.18488	1.76196
H	2.82517	-3.23407	-0.28480	H	2.90449	-1.46825	2.20774
H	1.21186	-2.67786	-0.76639	H	2.30703	0.19354	2.05170
H	2.60303	-2.38591	-1.82594	C	4.14284	-0.50917	0.03199
H	5.03776	-1.07562	0.31720	H	4.40951	0.39571	0.58649
H	4.66366	-0.09186	-1.10644	H	4.73574	-1.33426	0.44039
H	4.59632	0.62676	0.51382	H	4.43739	-0.37167	-1.01557
H	2.79764	2.32147	-0.42379	C	2.10680	1.62848	-0.39351
H	1.00254	3.72370	0.45343	H	3.14627	1.94193	-0.43244
H	-1.07926	2.52006	1.16469	C	-0.30052	2.11258	-0.11557
H	-1.23765	2.56495	-0.58998	H	-0.80456	2.29902	-1.07381
H	-2.01920	0.04050	-2.05830	H	-0.83865	2.68730	0.64633
H	-4.34620	-0.81570	-2.19582	C	1.14271	2.52527	-0.17919
H	-5.63218	-1.26283	-0.11831	H	1.39308	3.57384	-0.03777
H	-4.57773	-0.85341	2.09527	C	2.64871	-0.83779	0.15414
H	-2.25432	-0.00566	2.22371	H	2.12905	0.00574	-1.73370
Electronic Energy = -909.982549860				Electronic Energy = -658.5931436			
Zero-point corrected electronic energy=-909.677032				Zero-point corrected electronic energy=-658.275308			
Zero-point corrected Gibbs free energy=-909.70321				Zero-point corrected Gibbs free energy=-658.299122			
2a				2aC			
C	3.54205	-0.98156	-0.79900	C	3.22998	-1.31224	-0.82688
C	0.62412	-1.57606	-1.44265	C	0.76144	-1.49617	-1.12909
C	1.70483	-1.99492	1.44535	C	1.79443	-1.99099	1.09641
C	1.52638	0.90849	0.39005	C	1.79563	0.39246	0.30501
H	2.50039	1.15495	0.84446	H	2.76765	0.58863	0.78658
C	1.34332	1.80844	-0.79045	C	1.66829	1.36572	-0.83339
C	0.35152	2.69766	-0.88370	C	0.86152	2.42572	-0.79891
C	-0.64936	2.85170	0.22985	C	-0.02293	2.68393	0.38778
C	-0.71997	1.57372	1.06501	C	-0.33474	1.37833	1.11315
H	-1.19790	1.80460	2.02347	H	-0.68434	1.61432	2.12422
C	-1.52086	0.43712	0.43921	C	-1.40858	0.51350	0.46822
C	-1.75229	-0.69965	1.22330	C	-1.86619	-0.58502	1.20544
C	-2.51736	-1.75926	0.74355	C	-2.80811	-1.46227	0.67648
C	-3.07527	-1.69200	-0.53523	C	-3.31683	-1.24418	-0.60588
C	-2.85225	-0.56572	-1.32396	C	-2.88399	-0.14194	-1.33992
C	-2.07634	0.48974	-0.84077	C	-1.93544	0.73303	-0.80495
O	0.58799	1.15171	1.44844	O	0.85416	0.62145	1.35825
H	3.81715	-2.00796	-1.06476	H	3.35218	-2.37054	-1.07966
H	4.26920	-0.61694	-0.06591	H	4.05643	-1.02663	-0.16634

H	3.63517	-0.37058	-1.70348	H	3.32175	-0.74167	-1.75671
H	1.03401	-2.49971	-1.86658	H	0.94134	-2.51796	-1.48287
H	0.52389	-0.84541	-2.25279	H	0.74371	-0.83536	-2.00295
H	-0.37450	-1.78926	-1.05269	H	-0.22630	-1.47129	-0.66294
H	2.01606	-3.02101	1.22236	H	1.95051	-3.03745	0.81214
H	0.69098	-2.02579	1.85340	H	0.81893	-1.90183	1.58128
H	2.37231	-1.59496	2.21580	H	2.56485	-1.71641	1.82686
H	2.06922	1.70240	-1.59536	H	2.30667	1.19120	-1.69546
H	0.26119	3.33033	-1.76326	H	0.83580	3.12192	-1.63376
H	-1.64125	3.10784	-0.15623	H	-0.95277	3.17970	0.09186
H	-0.35319	3.67786	0.88754	H	0.48074	3.36209	1.08768
H	-1.32989	-0.74213	2.22470	H	-1.45776	-0.75796	2.19865
H	-2.68808	-2.63140	1.36781	H	-3.14461	-2.31408	1.25980
H	-3.67912	-2.51228	-0.91106	H	-4.04931	-1.92662	-1.02585
H	-3.27764	-0.50635	-2.32123	H	-3.27907	0.03650	-2.33553
H	-1.90323	1.35328	-1.47598	H	-1.59572	1.57498	-1.40108
Si	1.78431	-0.94053	-0.10864	C	1.86820	-1.09707	-0.14546
Electronic Energy = -909.980046084 Zero-point corrected electronic energy=-909.674133 Zero-point corrected Gibbs free energy=-909.69856				Electronic Energy = -658.58771294 Zero-point corrected electronic energy=-658.2698 Zero-point corrected Gibbs free energy=-658.292702			
2b				2bC			
C	-2.36601	-2.34765	-0.86402	C	-4.16227	-0.41974	-0.60919
Si	-2.74286	-0.69287	-0.05928	C	-2.33747	-2.11609	-0.69829
C	-2.53910	-0.79175	1.80542	C	-2.77340	-0.87067	1.43324
C	-4.47271	-0.11020	-0.51816	C	-1.75608	0.31087	-0.55746
C	-1.47025	0.58377	-0.71614	H	-1.81769	0.36120	-1.66170
H	-1.57700	0.66271	-1.81419	C	-2.03112	1.68334	0.00544
C	-1.67222	1.93382	-0.09944	C	-1.08047	2.42790	0.57341
C	-0.72021	2.55784	0.60012	C	0.35083	1.96700	0.63252
C	0.66341	1.97563	0.71054	C	0.55848	0.83374	-0.37566
C	0.87805	0.94924	-0.40518	H	0.48388	1.25203	-1.39361
H	0.89326	1.47687	-1.37302	C	1.90473	0.16989	-0.21200
C	2.17046	0.19068	-0.22949	C	3.04242	0.77689	-0.75148
C	3.35529	0.69524	-0.77136	C	4.30264	0.21080	-0.56673
C	4.56629	0.03521	-0.56529	C	4.43640	-0.97402	0.15798
C	4.60149	-1.14221	0.18175	C	3.30397	-1.58549	0.69477
C	3.42073	-1.65259	0.72208	C	2.04314	-1.01602	0.51261
C	2.21137	-0.98850	0.51999	O	-0.45653	-0.13975	-0.20050
O	-0.19615	0.01707	-0.40296	H	-4.85330	-1.23677	-0.37717
H	-3.04253	-3.12371	-0.49138	H	-4.55992	0.48729	-0.14444
H	-2.48034	-2.28925	-1.95130	H	-4.16242	-0.27875	-1.69630
H	-1.33811	-2.65262	-0.64521	H	-3.07204	-2.88722	-0.44268
H	-3.22178	-1.53234	2.23430	H	-2.27790	-2.05226	-1.79127
H	-1.51429	-1.08041	2.06066	H	-1.36036	-2.42859	-0.32158
H	-2.74615	0.17640	2.27265	H	-3.43752	-1.68193	1.75054
H	-5.21377	-0.86190	-0.22647	H	-1.76859	-1.07663	1.81467
H	-4.72939	0.82568	-0.01169	H	-3.13012	0.05857	1.88991

H	-4.56305	0.04861	-1.59786	H	-3.04691	2.06099	-0.07494
H	-2.65305	2.38790	-0.23059	H	-1.32548	3.40359	0.98689
H	-0.92142	3.51710	1.07039	H	1.03191	2.79533	0.40608
H	1.42124	2.76365	0.63143	H	0.60822	1.60839	1.63838
H	0.81403	1.48409	1.68149	H	2.94095	1.69639	-1.32427
H	3.32968	1.60833	-1.36197	H	5.17802	0.69007	-0.99446
H	5.48000	0.43615	-0.99344	H	5.41631	-1.41962	0.29867
H	5.54282	-1.65959	0.33919	H	3.40035	-2.51060	1.25533
H	3.44090	-2.57007	1.30255	H	1.15771	-1.49131	0.92310
H	1.28869	-1.38512	0.93306	C	-2.76061	-0.77044	-0.09532
Electronic Energy = -909.985102239 Zero-point corrected electronic energy=-909.679862 Zero-point corrected Gibbs free energy=-909.706306				Electronic Energy = -658.5961979 Zero-point corrected electronic energy=-658.279232 Zero-point corrected Gibbs free energy=-658.303233			
A Intermediates (Lithiated)							
Silicon analogues for deprotonated C^1				Carbon Analogues for deprotonated C^1			
1aA-C^1Li				1aCA-C^1Li			
C	-3.33950	-0.37429	1.76272	C	-2.21620	-2.00610	-0.38590
Si	-2.52431	-0.48336	0.06250	C	-3.53740	-0.04872	-1.20500
C	-1.06650	0.65365	0.03411	C	-3.51724	-0.61657	1.22429
O	-0.39357	0.72944	-1.21809	C	-1.46671	0.33882	0.11937
C	0.94751	1.20424	-1.15918	C	-1.12909	1.10153	1.18972
H	1.23740	1.33783	-2.20885	C	0.03701	1.98379	1.23302
C	1.86219	0.14196	-0.55572	C	0.42439	2.35355	-0.18901
C	1.45767	-1.19997	-0.55118	C	0.52451	1.07040	-1.03205
C	2.29517	-2.20072	-0.05170	H	0.72269	1.32431	-2.08133
C	3.55254	-1.87384	0.45318	C	1.64718	0.16808	-0.54647
C	3.96703	-0.54094	0.45704	C	1.39933	-1.12698	-0.08250
C	3.12787	0.45800	-0.03886	C	2.44470	-1.92760	0.39244
C	1.00710	2.55522	-0.42300	C	3.75309	-1.45101	0.38435
C	0.43338	2.38538	0.96388	C	4.01303	-0.16753	-0.10486
C	-0.69659	1.54784	1.02755	C	2.97030	0.63359	-0.56082
C	-2.05875	-2.28924	-0.27008	O	-0.71620	0.37315	-1.06232
C	-3.79606	-0.01756	-1.25648	H	-3.08759	-2.64144	-0.58274
H	-3.67369	0.64577	1.97929	H	-1.65870	-2.44634	0.44945
H	-2.65868	-0.68750	2.56137	H	-1.57854	-2.01508	-1.27498
H	-4.21738	-1.02856	1.79543	H	-4.40588	-0.70110	-1.35338
H	0.47853	-1.44823	-0.94571	H	-2.96523	-0.01672	-2.13603
H	1.96178	-3.23428	-0.06015	H	-3.89660	0.96255	-0.98626
H	4.20664	-2.64930	0.83957	H	-4.37016	-1.28557	1.06789
H	4.94603	-0.27570	0.84434	H	-3.90597	0.37437	1.48044
H	3.46764	1.48876	-0.02624	H	-2.94361	-0.99394	2.07788
H	0.43165	3.26312	-1.04106	H	-1.76494	1.01631	2.06921
H	2.03611	2.93101	-0.41689	H	-0.12084	2.85158	1.87954
H	0.55522	3.17912	1.69482	H	1.38007	2.88712	-0.25004
H	-1.27801	1.50456	1.95138	H	-0.32696	2.98880	-0.69508
H	-1.33326	-2.66145	0.46164	H	0.38436	-1.50884	-0.10347

H	-1.62635	-2.40910	-1.26986
H	-2.95126	-2.92385	-0.22003
H	-4.63764	-0.71966	-1.25411
H	-4.18770	0.99026	-1.08452
H	-3.34297	-0.03772	-2.25355
Li	0.97216	0.32271	1.72309

Electronic Energy = -916.931455656
Zero-point corrected electronic energy=-916.637372
Zero-point corrected Gibbs free energy=-916.662928

H	2.23243	-2.93003	0.75278
H	4.56633	-2.07418	0.74282
H	5.03156	0.20796	-0.13028
H	3.18425	1.63091	-0.93716
C	-2.66623	-0.57304	-0.04732
Li	1.05632	0.33031	2.05792

Electronic Energy = -665.53334445
Zero-point corrected electronic energy=-665.22792
Zero-point corrected Gibbs free energy=-665.251496

1bA-C[1]Li

C	4.41612	-0.03590	0.33565
Si	2.67620	-0.73842	0.12327
C	2.16311	-1.62116	1.72014
C	2.68803	-2.05959	-1.22990
C	1.53511	0.63384	-0.30826
C	1.64116	2.02174	-0.10544
C	0.55030	2.87713	-0.14897
C	-0.85398	2.33674	0.06175
C	-0.78276	0.82835	0.31155
H	-0.39211	0.65422	1.32635
C	-2.09653	0.09319	0.15197
C	-3.31003	0.70621	0.48376
C	-4.51387	0.01082	0.37313
C	-4.52356	-1.30843	-0.07824
C	-3.31931	-1.92677	-0.41293
C	-2.11563	-1.23201	-0.29632
O	0.17082	0.25257	-0.59961
H	5.13028	-0.84229	0.53438
H	4.74437	0.49079	-0.56675
H	4.45985	0.66597	1.17498
H	2.80040	-2.48940	1.92433
H	2.22177	-0.94108	2.57665
H	1.12812	-1.97505	1.64400
H	3.29546	-2.92281	-0.93569
H	1.67004	-2.41749	-1.42236
H	3.08851	-1.66155	-2.16834
H	2.64268	2.43581	0.01705
H	0.70519	3.94522	-0.03522
H	-1.31745	2.81605	0.93637
H	-1.53624	2.52848	-0.78130
H	-3.32135	1.73509	0.83152
H	-5.44508	0.50365	0.63621
H	-5.46098	-1.84867	-0.16815
H	-3.31527	-2.95414	-0.76503
H	-1.17849	-1.71240	-0.55820
Li	0.79263	1.45398	-2.09239

1bCA-C[1]Li

C	-2.48251	-0.58538	1.21006
C	-3.76932	-1.07464	0.98393
C	-4.39048	-0.86268	-0.24617
C	-3.71898	-0.15725	-1.24662
C	-2.43818	0.33824	-1.01309
C	-1.80569	0.12870	0.21835
H	-1.99717	-0.75918	2.16741
H	-4.28370	-1.62394	1.76659
H	-5.39024	-1.24584	-0.42606
H	-4.19550	0.00801	-2.20834
H	-1.91945	0.88660	-1.79499
C	-0.42544	0.66812	0.47065
H	-0.05179	0.28346	1.42873
O	0.46329	0.16234	-0.56408
C	1.83538	0.32426	-0.21729
C	2.53297	-1.77552	-1.37848
H	3.04446	-1.23666	-2.18394
H	3.01473	-2.75327	-1.25805
H	1.49357	-1.94113	-1.67884
C	1.95953	-1.81932	1.05241
H	0.90157	-2.00697	0.83647
H	2.46482	-2.78847	1.14511
H	2.02875	-1.29976	2.01448
C	4.05818	-0.69184	0.27926
H	4.15071	-0.19326	1.24982
H	4.61590	-1.63338	0.32856
H	4.52907	-0.05720	-0.48026
C	2.11368	1.59152	0.27057
H	3.14454	1.83026	0.52584
C	-0.32989	2.19286	0.46147
H	-0.98847	2.57761	-0.33314
H	-0.75936	2.56448	1.40483
C	1.13043	2.60209	0.30846
H	1.41809	3.57783	0.68667
C	2.59349	-0.97158	-0.06826
Li	1.29804	1.68889	-1.72993

Electronic Energy = -916.938242017 Zero-point corrected electronic energy=-916.644708 Zero-point corrected Gibbs free energy=-916.671397	Electronic Energy = -665.536607 Zero-point corrected electronic energy=-665.23123 Zero-point corrected Gibbs free energy=-665.255399
2aA-C[1]Li C 3.21114 -1.07708 -1.38742 C 0.65466 -2.34675 -0.28939 C 2.77099 -1.37121 1.65626 C 1.24186 0.72024 0.02905 C 1.12667 1.65369 -1.01163 C 0.31605 2.77746 -0.93012 C -0.81665 2.83897 0.08217 C -0.86546 1.56199 0.93211 H -1.25684 1.79284 1.92790 C -1.68927 0.42548 0.37076 C -2.32789 -0.44684 1.25881 C -3.07071 -1.52994 0.79180 C -3.18263 -1.75522 -0.58042 C -2.54988 -0.89201 -1.47436 C -1.80541 0.18881 -1.00278 O 0.49685 1.12330 1.19509 H 3.66945 -2.07195 -1.41223 H 4.00904 -0.33930 -1.25298 H 2.74570 -0.90211 -2.36334 H 1.09868 -3.34240 -0.17005 H 0.23944 -2.26983 -1.29996 H -0.18146 -2.25300 0.41337 H 3.14094 -2.40241 1.67683 H 2.06020 -1.25380 2.48175 H 3.61662 -0.69969 1.84006 H 1.74789 1.50064 -1.89510 H 0.29379 3.48119 -1.75629 H -1.78668 2.95766 -0.42343 H -0.73545 3.70134 0.75852 H -2.24296 -0.27116 2.32918 H -3.56312 -2.19381 1.49625 H -3.76114 -2.59689 -0.94953 H -2.63182 -1.06343 -2.54387 H -1.31341 0.86027 -1.70134 Si 1.93491 -0.98318 0.00430 Li 1.90227 2.55281 0.85148 Electronic Energy = -916.93886165 Zero-point corrected electronic energy=-916.644787 Zero-point corrected Gibbs free energy=-916.669904	2aCA-C[1]Li C 2.40137 -1.68849 -1.37963 C 0.53061 -2.14450 0.21492 C 2.79805 -1.58224 1.08579 C 1.44485 0.18375 -0.04825 C 1.50599 1.12294 -1.05167 C 1.07022 2.45798 -0.85101 C -0.02207 2.72894 0.18254 C -0.34441 1.45878 0.98002 H -0.62632 1.71314 2.00587 C -1.43273 0.58225 0.40476 C -2.19502 -0.20400 1.27429 C -3.16953 -1.07357 0.78876 C -3.39714 -1.16386 -0.58510 C -2.65110 -0.37563 -1.46117 C -1.67364 0.49035 -0.97013 O 0.88985 0.68817 1.15798 H 2.69148 -2.74438 -1.35328 H 3.29725 -1.09732 -1.60048 H 1.68806 -1.55144 -2.19950 H 0.79519 -3.20916 0.21820 H -0.22736 -1.97070 -0.55644 H 0.08471 -1.89861 1.18331 H 3.00322 -2.65744 1.15538 H 2.40698 -1.24720 2.05186 H 3.74552 -1.06455 0.89615 H 1.97750 0.84854 -1.99302 H 1.10703 3.12725 -1.70551 H -0.95407 3.07856 -0.28867 H 0.25164 3.51874 0.89578 H -2.01398 -0.13841 2.34522 H -3.75147 -1.67733 1.47876 H -4.15458 -1.84035 -0.96952 H -2.82719 -0.43811 -2.53111 H -1.09068 1.10097 -1.65412 Li 2.52643 1.86900 0.69067 C 1.78439 -1.28680 -0.03657 Electronic Energy = -665.535217312 Zero-point corrected electronic energy=-665.225991 Zero-point corrected Gibbs free energy=-665.251137
2bA-C[1]Li	2bCA-C[1]Li

C	4.46588	0.13833	0.02253
Si	2.79571	-0.74203	0.09640
C	1.45226	0.50961	-0.06200
O	0.13833	-0.05037	-0.06734
C	-0.90353	0.84982	0.27843
H	-0.78213	1.16149	1.33338
C	-2.21513	0.11289	0.17007
C	-3.22784	0.32128	1.10876
C	-4.46253	-0.31496	0.97698
C	-4.69300	-1.17351	-0.09709
C	-3.68402	-1.38894	-1.03758
C	-2.45377	-0.74677	-0.90689
C	-0.87841	2.10424	-0.62073
C	0.49946	2.71959	-0.60580
C	1.57315	1.83927	-0.46749
C	2.67520	-1.70550	1.72093
C	2.73029	-2.02711	-1.29177
H	4.60576	0.64730	-0.93694
H	4.57177	0.88011	0.82125
H	5.27494	-0.59173	0.13458
H	-3.04809	0.98487	1.95189
H	-5.23976	-0.14584	1.71615
H	-5.65118	-1.67351	-0.20041
H	-3.85718	-2.05857	-1.87491
H	-1.66423	-0.91411	-1.63386
H	-1.19486	1.77700	-1.62562
H	-1.65273	2.79675	-0.26445
H	0.64991	3.72371	-0.98820
H	2.59187	2.22695	-0.54750
H	2.84299	-1.05180	2.58372
H	1.68306	-2.15762	1.82738
H	3.41642	-2.51219	1.75462
H	3.49868	-2.79726	-1.15937
H	2.88124	-1.55293	-2.26724
H	1.75377	-2.52344	-1.30780
Li	1.26836	2.38092	1.58079

Electronic Energy = -916.9268778
Zero-point corrected electronic energy=-916.633751
Zero-point corrected Gibbs free energy=-916.660717

C	4.13914	-0.52957	-0.22601
C	1.74369	0.23509	-0.08005
O	0.44005	-0.16822	0.21981
C	-0.55823	0.84513	0.29200
H	-0.48579	1.34013	1.27499
C	-1.90065	0.16102	0.18610
C	-3.01319	0.68412	0.84972
C	-4.27130	0.10078	0.69927
C	-4.42817	-1.01934	-0.11706
C	-3.32049	-1.54986	-0.77925
C	-2.06464	-0.96235	-0.62954
C	-0.36142	1.90707	-0.80103
C	1.00447	2.55444	-0.64190
C	2.01289	1.49359	-0.49917
C	2.66962	-1.34444	1.62045
C	2.27336	-2.10993	-0.72925
H	4.21788	-0.23830	-1.27867
H	4.50110	0.30125	0.38931
H	4.80161	-1.38565	-0.05903
H	-2.89360	1.55506	1.49107
H	-5.12670	0.51739	1.22292
H	-5.40562	-1.47748	-0.23355
H	-3.43463	-2.42345	-1.41461
H	-1.19613	-1.37350	-1.13593
H	-0.48532	1.36987	-1.76275
H	-1.19161	2.62187	-0.73059
H	1.24301	3.22790	-1.47247
H	3.05662	1.72468	-0.70577
H	3.01658	-0.53005	2.26665
H	1.65299	-1.61406	1.91939
H	3.32025	-2.21171	1.78396
H	2.94153	-2.96332	-0.56426
H	2.30865	-1.84215	-1.79098
H	1.25246	-2.41710	-0.48528
Li	1.53632	3.28631	1.27007
C	2.70448	-0.91483	0.14186

Electronic Energy = -665.530406399
Zero-point corrected electronic energy=-665.225991
Zero-point corrected Gibbs free energy=-665.5304064

Silicon analogues for deprotonated C^2			
1aA-C^2Li			
C	2.71995	-2.06545	1.02088
Si	2.72856	-0.52393	-0.06121
C	3.63331	0.88390	0.79966
C	3.54968	-0.90785	-1.71447
C	0.91887	-0.00593	-0.37018

Carbon analogues for deprotonated C^2			
1aCA-C^2Li			
C	2.34338	-1.97586	0.77216
C	3.56831	0.20872	0.69055
C	3.23775	-1.14177	-1.39623
C	1.25720	-0.01156	-0.32046
H	0.62523	-0.73328	-0.87203

H	0.40805	-0.85431	-0.86556	C	1.36477	1.24797	-1.14516
C	0.81867	1.19792	-1.25920	C	0.66657	2.34738	-0.85395
C	0.14321	2.29623	-0.90672	C	-0.29858	2.38799	0.30812
C	-0.64619	2.34326	0.38334	C	-0.58051	1.00012	0.85500
C	-0.90303	0.94806	0.92710	C	-1.67201	0.22572	0.30190
C	-1.98796	0.17519	0.34185	C	-1.64912	-1.20196	0.32653
C	-1.94069	-1.24835	0.30109	C	-2.73278	-1.96629	-0.08820
C	-3.01480	-2.01231	-0.14142	C	-3.90867	-1.36959	-0.55588
C	-4.20041	-1.41271	-0.57702	C	-3.95852	0.02744	-0.59569
C	-4.27070	-0.01614	-0.56021	C	-2.88101	0.80477	-0.18562
C	-3.20155	0.75720	-0.12156	O	0.65442	0.26284	0.94191
O	0.35388	0.22213	0.92787	H	3.27958	-2.51552	0.95432
H	3.73897	-2.41596	1.21527	H	1.65925	-2.65265	0.24538
H	2.16900	-2.87661	0.53269	H	1.89515	-1.71760	1.73484
H	2.23901	-1.85771	1.98157	H	4.50953	-0.31170	0.90169
H	4.67727	0.61886	0.99686	H	3.12784	0.52859	1.63931
H	3.15206	1.12005	1.75381	H	3.80003	1.10323	0.10204
H	3.62022	1.78731	0.18097	H	4.12630	-1.75435	-1.20729
H	4.56168	-1.29647	-1.55843	H	3.55256	-0.28368	-1.99763
H	3.62718	-0.01116	-2.33791	H	2.53748	-1.73951	-1.99169
H	2.98280	-1.66148	-2.27142	H	2.02755	1.23463	-2.00768
H	1.33999	1.14769	-2.21547	H	0.79970	3.24928	-1.45139
H	0.14856	3.17008	-1.55734	H	-1.22296	2.88270	-0.00900
H	-1.58683	2.87852	0.21528	H	0.12854	3.04989	1.07887
H	-0.09528	2.95539	1.11457	H	-0.75165	-1.69610	0.68909
H	-1.03482	-1.74532	0.63812	H	-2.65660	-3.05098	-0.04981
H	-2.92286	-3.09630	-0.15016	H	-4.75211	-1.96994	-0.88060
H	-5.03708	-2.01109	-0.92265	H	-4.85421	0.52473	-0.96186
H	-5.17469	0.48271	-0.90292	H	-2.97796	1.88567	-0.23551
H	-3.31123	1.83790	-0.12655	Li	-1.42756	0.88896	2.82843
Li	-1.41433	0.59591	2.99148	C	2.60889	-0.71691	-0.06335
Electronic Energy = -916.931455656 Zero-point corrected electronic energy=-916.624653 Zero-point corrected Gibbs free energy=-916.65118				Electronic Energy = -665.528147863 Zero-point corrected electronic energy=-665.224309 Zero-point corrected Gibbs free energy=-665.248781			
1bA-C^2Li				1bCA-C^2Li			
C	4.41612	-0.03590	0.33565	C	-2.87067	0.95483	0.28803
Si	2.67620	-0.73842	0.12327	C	-4.12299	0.35515	0.36408
C	2.16311	-1.62116	1.72014	C	-4.30678	-0.99689	0.05512
C	2.68803	-2.05959	-1.22990	C	-3.18719	-1.73357	-0.35240
C	1.53511	0.63384	-0.30826	C	-1.92717	-1.15612	-0.43289
C	1.64116	2.02174	-0.10544	C	-1.70575	0.21618	-0.09441
C	0.55030	2.87713	-0.14897	H	-2.78529	2.01581	0.50844
C	-0.85398	2.33674	0.06175	H	-4.97774	0.96243	0.65407
C	-0.78276	0.82835	0.31155	H	-5.28894	-1.45437	0.11056
H	-0.39211	0.65422	1.32635	H	-3.30302	-2.78100	-0.62331
C	-2.09653	0.09319	0.15197	H	-1.07821	-1.74513	-0.76535

C	-3.31003	0.70621	0.48376
C	-4.51387	0.01082	0.37313
C	-4.52356	-1.30843	-0.07824
C	-3.31931	-1.92677	-0.41293
C	-2.11563	-1.23201	-0.29632
O	0.17082	0.25257	-0.59961
H	5.13028	-0.84229	0.53438
H	4.74437	0.49079	-0.56675
H	4.45985	0.66597	1.17498
H	2.80040	-2.48940	1.92433
H	2.22177	-0.94108	2.57665
H	1.12812	-1.97505	1.64400
H	3.29546	-2.92281	-0.93569
H	1.67004	-2.41749	-1.42236
H	3.08851	-1.66155	-2.16834
H	2.64268	2.43581	0.01705
H	0.70519	3.94522	-0.03522
H	-1.31745	2.81605	0.93637
H	-1.53624	2.52848	-0.78130
H	-3.32135	1.73509	0.83152
H	-5.44508	0.50365	0.63621
H	-5.46098	-1.84867	-0.16815
H	-3.31527	-2.95414	-0.76503
H	-1.17849	-1.71240	-0.55820
Li	0.79263	1.45398	-2.09239

Electronic Energy = -916.910976268
Zero-point corrected electronic energy=-916.617746
Zero-point corrected Gibbs free energy=-916.643263

C	-0.39195	0.77630	-0.05421
Li	-0.62044	0.35733	2.06555
O	0.50861	0.05245	-0.91334
C	1.89187	0.25437	-0.69046
C	2.37868	-2.19064	-0.63683
H	2.95064	-2.14424	-1.57084
H	2.75220	-3.03931	-0.05278
H	1.32952	-2.37514	-0.88681
C	1.81670	-1.04848	1.50199
H	0.78132	-1.36628	1.33406
H	2.31372	-1.81998	2.10117
H	1.83332	-0.11114	2.07044
C	4.01252	-0.60349	0.38606
H	4.16655	0.22419	1.08569
H	4.50023	-1.49061	0.80461
H	4.51868	-0.35587	-0.55499
C	2.20380	1.66304	-0.25151
H	3.25531	1.92506	-0.16079
C	-0.20039	2.26460	-0.23216
H	-0.58114	2.63234	-1.20822
H	-0.75135	2.82923	0.53000
C	1.26223	2.60061	-0.11712
H	1.54716	3.63168	0.08545
C	2.52305	-0.88563	0.15608
H	2.35356	0.14906	-1.68746

Electronic Energy = -665.528147863
Zero-point corrected electronic energy=-665.216965
Zero-point corrected Gibbs free energy=-665.240426

2aA-C^2Li

C	3.78513	-0.95685	-0.84575
C	0.83332	-0.98654	-1.72311
C	1.75688	-2.55531	0.80482
C	1.75642	0.53910	0.86289
H	2.37414	0.38909	1.76054
C	2.19359	1.79194	0.16875
C	1.32252	2.67040	-0.33634
C	-0.16938	2.46907	-0.27539
C	-0.54991	1.20197	0.43165
C	-1.66810	0.41664	0.17526
C	-1.86379	-0.89243	0.75123
C	-3.01118	-1.63419	0.50722
C	-4.04286	-1.16237	-0.31434
C	-3.87158	0.10572	-0.89817
C	-2.74452	0.87445	-0.67272
O	0.40823	0.67717	1.35147
H	4.03850	-1.88311	-1.37242
H	4.48284	-0.84564	-0.00846

2aCA-C^2Li

C	2.34338	-1.97586	0.77216
C	3.56831	0.20872	0.69055
C	3.23775	-1.14177	-1.39623
C	1.25720	-0.01156	-0.32046
H	0.62523	-0.73328	-0.87203
C	1.36477	1.24797	-1.14516
C	0.66657	2.34738	-0.85395
C	-0.29858	2.38799	0.30812
C	-0.58051	1.00012	0.85500
C	-1.67201	0.22572	0.30190
C	-1.64912	-1.20196	0.32653
C	-2.73278	-1.96629	-0.08820
C	-3.90867	-1.36959	-0.55588
C	-3.95852	0.02744	-0.59569
C	-2.88101	0.80477	-0.18562
O	0.65442	0.26284	0.94191
H	3.27958	-2.51552	0.95432
H	1.65925	-2.65265	0.24538

H	3.94526	-0.12254	-1.53629
H	1.12193	-1.76686	-2.43649
H	0.88275	-0.01804	-2.23346
H	-0.20217	-1.15592	-1.41391
H	1.94196	-3.45527	0.20855
H	0.74038	-2.62050	1.20317
H	2.45851	-2.55865	1.64593
H	3.26542	1.95407	0.07293
H	1.68352	3.57267	-0.82564
H	-0.54114	2.43122	-1.31169
H	-0.62464	3.38253	0.15088
H	-1.07675	-1.31310	1.37061
H	-3.09782	-2.61885	0.96425
H	-4.93291	-1.75313	-0.50099
H	-4.64759	0.50341	-1.55007
H	-2.67195	1.85414	-1.13718
Li	-0.90153	1.16625	2.60308
Si	1.99567	-1.01294	-0.24909

Electronic Energy = -916.917552266
Zero-point corrected electronic energy=-916.625783
Zero-point corrected Gibbs free energy=-916.651925

H	1.89515	-1.71760	1.73484
H	4.50953	-0.31170	0.90169
H	3.12784	0.52859	1.63931
H	3.80003	1.10323	0.10204
H	4.12630	-1.75435	-1.20729
H	3.55256	-0.28368	-1.99763
H	2.53748	-1.73951	-1.99169
H	2.02755	1.23463	-2.00768
H	0.79970	3.24928	-1.45139
H	-1.22296	2.88270	-0.00900
H	0.12854	3.04989	1.07887
H	-0.75165	-1.69610	0.68909
H	-2.65660	-3.05098	-0.04981
H	-4.75211	-1.96994	-0.88060
H	-4.85421	0.52473	-0.96186
H	-2.97796	1.88567	-0.23551
Li	-1.42756	0.88896	2.82843
C	2.60889	-0.71691	-0.06335

Electronic Energy = -665.527323969
Zero-point corrected electronic energy=-665.223372
Zero-point corrected Gibbs free energy=-665.247181

2bA-C²Li

C	3.35411	0.83861	0.15846
C	4.55958	0.16352	0.31569
C	4.62762	-1.22911	0.20617
C	3.44528	-1.92786	-0.05441
C	2.23392	-1.26201	-0.21463
C	2.14375	0.15335	-0.13447
H	3.34522	1.92079	0.26025
H	5.45909	0.73241	0.53952
H	5.56953	-1.75252	0.33517
H	3.46523	-3.01327	-0.12431
H	1.32669	-1.82654	-0.40449
C	0.89868	0.86187	-0.38157
Li	1.21215	1.27382	-2.48999
O	-0.21404	-0.03961	-0.15573
C	-1.44379	0.43381	-0.66697
C	-4.45119	-0.25288	-0.68146
H	-4.41680	-0.35481	-1.77149
H	-5.23508	-0.91982	-0.30708
H	-4.74672	0.77455	-0.44475
C	-2.84768	-0.40963	1.95413
H	-3.14019	0.62022	2.18333
H	-3.56759	-1.08465	2.42884
H	-1.86256	-0.58824	2.39607
C	-2.34309	-2.47564	-0.29469
H	-1.36757	-2.72181	0.13595

2bCA-C²Li

C	3.04870	0.93414	0.06685
C	4.29915	0.33797	0.18901
C	4.44245	-1.05302	0.17309
C	3.28887	-1.83247	0.04222
C	2.03280	-1.24813	-0.08436
C	1.86421	0.16369	-0.09788
H	2.98086	2.01863	0.09681
H	5.17574	0.97013	0.31215
H	5.41950	-1.51392	0.27628
H	3.36858	-2.91733	0.04888
H	1.15000	-1.87402	-0.17216
C	0.57244	0.78091	-0.32300
Li	0.89292	0.84965	-2.46465
O	-0.47669	-0.13856	0.04768
C	-1.73289	0.20166	-0.48831
C	-4.12162	-0.58262	-0.64905
H	-4.00576	-0.68762	-1.73445
H	-4.84197	-1.33709	-0.31458
H	-4.55783	0.39985	-0.44469
C	-2.97025	-0.58665	1.58000
H	-3.37537	0.40657	1.80148
H	-3.66796	-1.33337	1.97579
H	-2.01473	-0.69087	2.10211
C	-2.29427	-2.21538	-0.19772
H	-1.35850	-2.41291	0.33092

H	-3.08591	-3.16840	0.11395	H	-3.04521	-2.94157	0.13295
H	-2.28809	-2.63527	-1.37691	H	-2.12099	-2.37107	-1.26988
C	-1.67762	1.88062	-0.33340	C	-2.05563	1.65248	-0.21212
H	-2.66765	2.28927	-0.53629	H	-3.08101	1.98566	-0.35732
C	0.66459	2.11069	0.45747	C	0.31890	2.10835	0.37287
H	0.81986	1.91757	1.53977	H	0.56489	2.06937	1.45484
H	1.37567	2.90342	0.19377	H	0.94861	2.90472	-0.04305
C	-0.73323	2.63327	0.24180	C	-1.12452	2.50946	0.21527
H	-0.95965	3.65486	0.54317	H	-1.40187	3.53610	0.45070
H	-1.47762	0.30432	-1.77060	C	-2.78364	-0.78717	0.07229
Si	-2.78968	-0.69059	0.09636	H	-1.71047	0.04892	-1.58920
Electronic Energy=-916.9170161 Zero-point corrected electronic energy= -916.62534 Zero-point corrected Gibbs free energy = -916.651636				Electronic Energy = -665.529000932 Zero-point corrected electronic energy=-665.224729 Zero-point corrected Gibbs free energy=-665.248644			
A Intermediates (Anionic)							
Silicon analogues for deprotonated C[1]				Carbon Analogues for deprotonated C[1]			
1-Anionic				1C-Anionic			
C	-2.01945	-2.22614	-0.45419	C	-2.05798	-2.01495	-0.38707
C	-3.86990	0.05712	-1.04421	C	-3.58819	-0.09171	-0.80492
C	-3.12210	-0.54761	1.85546	C	-3.08307	-0.80576	1.53106
C	-1.02696	0.71734	0.05612	C	-1.32029	0.33402	0.15848
C	-0.57007	1.53436	1.09723	C	-0.95381	1.20900	1.15284
C	0.45024	2.46444	0.98411	C	-0.09311	2.32309	0.96889
C	1.09233	2.60963	-0.36777	C	0.41418	2.48841	-0.44001
C	0.99719	1.26152	-1.10816	C	0.53177	1.10567	-1.12092
H	1.32496	1.38706	-2.14984	H	0.78208	1.22201	-2.18549
C	1.84474	0.15475	-0.49198	C	1.58723	0.19998	-0.49869
C	1.42032	-1.17282	-0.60770	C	1.43760	-1.18867	-0.57390
C	2.20371	-2.22377	-0.12991	C	2.42377	-2.04780	-0.08806
C	3.43281	-1.96217	0.47646	C	3.58556	-1.52823	0.48500
C	3.86443	-0.64219	0.60338	C	3.74633	-0.14610	0.56763
C	3.07247	0.40606	0.12910	C	2.75112	0.70887	0.08589
O	-0.36791	0.87546	-1.21334	O	-0.74781	0.48667	-1.13113
H	-2.91859	-2.85334	-0.41050	H	-2.92222	-2.68924	-0.44391
H	-1.25339	-2.67413	0.18849	H	-1.31098	-2.46246	0.27807
H	-1.65204	-2.25037	-1.48709	H	-1.62367	-1.93357	-1.38855
H	-4.66655	-0.69747	-1.04963	H	-4.43031	-0.79403	-0.86966
H	-3.51920	0.18427	-2.07514	H	-3.18955	0.06227	-1.81247
H	-4.29955	1.01140	-0.71930	H	-3.96480	0.86879	-0.43616
H	-3.98130	-1.22794	1.87806	H	-3.91000	-1.52446	1.49208
H	-3.46025	0.43210	2.20945	H	-3.47451	0.13980	1.92016
H	-2.37329	-0.92415	2.56046	H	-2.33462	-1.18323	2.23677
H	-1.04799	1.38784	2.06796	H	-1.35473	1.01335	2.14726
H	0.81779	3.01818	1.84197	H	0.52555	2.65818	1.79970
H	2.13815	2.93725	-0.30766	H	1.37097	3.02317	-0.48883
H	0.59289	3.34466	-1.02213	H	-0.27237	3.05866	-1.08821
H	0.46024	-1.36622	-1.07287	H	0.53073	-1.58666	-1.01579

H	1.85155	-3.24713	-0.22966
H	4.04706	-2.77763	0.84749
H	4.81768	-0.42471	1.07710
H	3.42310	1.42646	0.24805
Si	-2.42689	-0.44807	0.09456

Electronic Energy = -909.440374981
Zero-point corrected electronic energy=-909.149383
Zero-point corrected Gibbs free energy=-909.174131

H	2.28376	-3.12336	-0.15516
H	4.35580	-2.19388	0.86390
H	4.64479	0.27198	1.01304
H	2.88997	1.78180	0.17209
C	-2.48335	-0.62957	0.13216

Electronic Energy = -658.0330512
Zero-point corrected electronic energy=-657.730792
Zero-point corrected Gibbs free energy=-657.754141

2-Anionic

C	-2.55476	-0.40743	-1.07104
C	-3.80506	-1.00764	-1.21530
C	-4.66894	-1.10439	-0.12289
C	-4.27039	-0.60223	1.11612
C	-3.01556	-0.00860	1.25800
C	-2.14589	0.09764	0.16912
H	-1.87609	-0.33361	-1.91627
H	-4.10864	-1.39875	-2.18231
H	-5.64390	-1.56893	-0.23683
H	-4.93374	-0.67588	1.97312
H	-2.70426	0.37780	2.22599
C	-0.82155	0.79868	0.30479
H	-0.54351	0.85352	1.37109
O	0.16386	0.04591	-0.39059
C	1.48867	0.57391	-0.21916
Si	2.79605	-0.66155	0.05461
C	2.93319	-1.92878	-1.35780
H	3.21476	-1.43549	-2.29466
H	3.67822	-2.70248	-1.13542
H	1.96945	-2.42565	-1.51893
C	2.54659	-1.72084	1.61802
H	1.54021	-2.15574	1.62076
H	3.26967	-2.54365	1.67807
H	2.64509	-1.10765	2.52073
C	4.47552	0.20418	0.20741
H	4.49998	0.87583	1.07215
H	5.27084	-0.53921	0.33503
H	4.70442	0.79312	-0.68730
C	1.58114	1.96997	-0.14115
H	2.58394	2.37879	0.00084
C	-0.87285	2.23546	-0.25796
H	-1.29560	2.15407	-1.27612
H	-1.60502	2.81289	0.32705
C	0.50455	2.83825	-0.19902
H	0.63051	3.90642	-0.05165

Electronic Energy = -909.442399035

2C-Anionic

C	2.78032	0.25488	-1.20803
C	4.06160	-0.27811	-1.06808
C	4.42465	-0.92573	0.11386
C	3.49780	-1.03125	1.15214
C	2.21975	-0.49156	1.01124
C	1.84436	0.15536	-0.17327
H	2.49874	0.75376	-2.13289
H	4.77441	-0.19359	-1.88337
H	5.41974	-1.34627	0.22418
H	3.77193	-1.53646	2.07409
H	1.49237	-0.57947	1.81312
C	0.48672	0.78304	-0.29827
H	0.25778	0.96229	-1.36240
O	-0.47249	-0.12498	0.23238
C	-1.80089	0.33048	0.08188
C	-2.70148	-1.76577	1.10544
H	-3.01354	-1.24287	2.01631
H	-3.35708	-2.63475	0.96059
H	-1.67841	-2.12639	1.25077
C	-2.39368	-1.62028	-1.36847
H	-1.35695	-1.96518	-1.30574
H	-3.04399	-2.49771	-1.48212
H	-2.49482	-0.99565	-2.26326
C	-4.20202	-0.30957	-0.25684
H	-4.30535	0.33580	-1.13624
H	-4.88469	-1.15908	-0.37557
H	-4.51617	0.26032	0.62414
C	-2.03043	1.67987	0.12209
H	-3.05076	2.01249	-0.06764
C	0.37814	2.13080	0.46017
H	0.73096	1.90755	1.48426
H	1.11119	2.83441	0.03859
C	-1.03288	2.66266	0.38650
H	-1.17880	3.64900	-0.05302
C	-2.76473	-0.81455	-0.10751

Electronic Energy = -658.036108643

Zero-point corrected electronic energy=-909.152117 Zero-point corrected Gibbs free energy=-909.178325	Zero-point corrected electronic energy=-657.734764 Zero-point corrected Gibbs free energy=-657.758786
Silicon analogues for deprotonated C^2	Carbon analogues for deprotonated C^2
1-Anionic H -3.13476 -2.60743 -0.99478 C -3.03612 -1.61783 -0.54764 C -1.90388 -0.87926 -0.83687 H -1.14648 -1.28715 -1.49905 C -1.68029 0.44281 -0.27244 C -0.52987 1.15999 -0.48912 C -2.78398 0.93561 0.53960 H -2.73334 1.94028 0.95142 C -3.89817 0.16312 0.80799 H -4.68077 0.58941 1.43593 C -4.06137 -1.13732 0.29092 H -4.94527 -1.72803 0.50690 O 0.41770 0.65644 -1.40888 C -0.23197 2.53564 0.02048 C 1.24990 2.75479 0.19567 H -0.71665 2.68604 0.99504 H -0.62899 3.34652 -0.62562 C 2.14694 1.84206 -0.19136 H 1.57911 3.68500 0.65650 C 1.74089 0.56762 -0.87051 H 3.21203 2.00079 -0.02786 Si 1.98917 -0.97806 0.24211 C 3.77634 -0.92371 0.85992 C 1.76589 -2.51434 -0.82644 C 0.82131 -1.03320 1.71222 H 4.48188 -0.80400 0.03008 H 4.03030 -1.85098 1.38519 H 3.92669 -0.09133 1.55559 H 0.90122 -0.11893 2.30986 H 1.06670 -1.88864 2.35292 H -0.21403 -1.12593 1.36978 H 2.44436 -2.49588 -1.68613 H 0.73968 -2.57677 -1.20060 H 1.97282 -3.42172 -0.24854 H 2.40170 0.41427 -1.73983 Electronic Energy = -909.427678522 Zero-point corrected electronic energy=-909.138648 Zero-point corrected Gibbs free energy=-909.164562	1C-Anionic C -3.67762 -0.95640 0.70580 C -1.29166 -1.01898 1.46127 C -1.99782 -2.26348 -0.59004 C -1.93779 0.23441 -0.67044 H -2.57459 0.08769 -1.55923 C -2.32800 1.56294 -0.07504 C -1.45151 2.54779 0.12922 C 0.02127 2.36839 -0.12127 C 0.35388 0.94148 -0.41194 C 1.57360 0.34265 -0.21857 C 1.84761 -1.03519 -0.59899 C 3.06345 -1.64026 -0.33985 C 4.12839 -0.96476 0.28759 C 3.91145 0.38760 0.61910 C 2.71333 1.03119 0.37368 O -0.61357 0.25396 -1.18603 H -3.93647 -1.90227 1.19506 H -4.36335 -0.81821 -0.13995 H -3.85341 -0.15033 1.42520 H -1.55446 -1.87118 2.10072 H -1.39573 -0.10169 2.05126 H -0.24462 -1.11398 1.15912 H -2.15384 -3.15520 0.02801 H -0.98109 -2.29378 -0.98974 H -2.70026 -2.30702 -1.43164 H -3.38619 1.71929 0.12237 H -1.79631 3.51741 0.48596 H 0.56516 2.70338 0.77160 H 0.32301 3.07513 -0.92432 H 1.06323 -1.59453 -1.09846 H 3.19659 -2.67923 -0.64272 H 5.07826 -1.45235 0.47930 H 4.71914 0.96005 1.07580 H 2.62362 2.08328 0.63217 C -2.21526 -0.99373 0.24076 Electronic Energy = -658.040475459 Zero-point corrected electronic energy=-657.739369 Zero-point corrected Gibbs free energy=-657.762899
2-Anionic	2C-Anionic

C	3.77542	-0.92513	-0.86041
C	0.82016	-1.03300	-1.71201
C	1.76461	-2.51438	0.82621
C	1.74123	0.56761	0.87075
H	2.40224	0.41408	1.73988
C	2.14756	1.84183	0.19141
C	1.25062	2.75450	-0.19598
C	-0.23128	2.53544	-0.02108
C	-0.52944	1.16018	0.48954
C	-1.67982	0.44304	0.27281
C	-1.90391	-0.87882	0.83752
C	-3.03609	-1.61732	0.54792
C	-4.06095	-1.13688	-0.29117
C	-3.89744	0.16350	-0.80832
C	-2.78331	0.93592	-0.53957
O	0.41818	0.65677	1.40932
H	4.02989	-1.85403	-1.38250
H	4.48110	-0.80173	-0.03122
H	3.92506	-0.09498	-1.55893
H	1.06803	-1.88631	-2.35460
H	0.89696	-0.11727	-2.30779
H	-0.21476	-1.12970	-1.36935
H	1.96277	-3.42194	0.24546
H	0.74067	-2.57231	1.20726
H	2.44924	-2.50086	1.68110
H	3.21269	2.00030	0.02794
H	1.57992	3.68458	-0.65700
H	-0.71545	2.68490	-0.99605
H	-0.62877	3.34685	0.62402
H	-1.14680	-1.28672	1.50003
H	-3.13505	-2.60681	0.99525
H	-4.94478	-1.72758	-0.50742
H	-4.67980	0.58983	-1.43653
H	-2.73246	1.94062	-0.95132
Si	1.98855	-0.97814	-0.24205

Electronic Energy = -909.42767823
Zero-point corrected electronic energy =-909.138664
Zero-point corrected Gibbs free energy =-909.164599

C	-2.71332	1.03116	0.37403
C	-3.91155	0.38763	0.61898
C	-4.12850	-0.96468	0.28714
C	-3.06342	-1.64020	-0.33993
C	-1.84745	-1.03513	-0.59864
C	-1.57352	0.34268	-0.21818
H	-2.62366	2.08320	0.63270
H	-4.71933	0.96001	1.07561
H	-5.07847	-1.45220	0.47860
H	-3.19646	-2.67916	-0.64288
H	-1.06299	-1.59448	-1.09797
C	-0.35387	0.94155	-0.41170
O	0.61349	0.25418	-1.18613
C	1.93769	0.23428	-0.67046
C	1.99750	-2.26357	-0.59000
H	2.70024	-2.30743	-1.43134
H	2.15302	-3.15526	0.02822
H	0.98091	-2.29367	-0.99010
C	1.29178	-1.01895	1.46146
H	0.24469	-1.11441	1.15968
H	1.55505	-1.87090	2.10107
H	1.39580	-0.10147	2.05114
C	3.67755	-0.95644	0.70550
H	3.85337	-0.15059	1.42516
H	3.93667	-1.90245	1.19433
H	4.36305	-0.81779	-0.14036
C	2.32810	1.56274	-0.07500
H	3.38630	1.71894	0.12249
C	-0.02109	2.36850	-0.12151
H	-0.32221	3.07491	-0.92514
H	-0.56520	2.70418	0.77094
C	1.45172	2.54768	0.12926
H	1.79662	3.51725	0.48605
C	2.21508	-0.99382	0.24074
H	2.57447	0.08741	-1.55925

Electronic Energy = -658.040426784
Zero-point corrected electronic energy=-657.739438
Zero-point corrected Gibbs free energy=-657.763239

15. Cartesian coordinates for optimized geometries of the C^1 proton abstraction transition states of 2-silyl-6-aryl-5,6-dihydro-(2H)-pyranstereomers in THF solvent at 195 K.

1a-TS- C^1			
C	0.34585	-1.31876	1.55590

1b-TS- C^1			
C	2.89441	-2.67666	-0.24899

C	-0.65589	-2.18318	1.81309	Si	1.44360	-1.60468	-0.80344
C	0.63068	-0.72228	0.25751	C	0.12343	-2.71202	-1.58947
H	0.99940	-0.99469	2.36675	C	2.02548	-0.40858	-2.14165
O	-0.30116	-1.15175	-0.80882	C	0.77996	-0.66056	0.67709
H	0.40362	0.64156	0.18052	H	1.47314	0.45548	1.03301
Si	2.35281	-1.19668	-0.34176	C	0.63563	-1.39059	1.93398
C	-1.54345	-2.65264	0.69293	C	-0.47274	-1.38418	2.70267
H	-0.83277	-2.55458	2.81834	C	-1.74981	-0.76063	2.19843
C	-1.61047	-1.63319	-0.44870	C	-1.66855	-0.61711	0.67999
H	-1.17093	-3.59882	0.27566	H	-1.62402	-1.62221	0.23866
H	-2.56366	-2.84807	1.04266	C	-2.81578	0.13681	0.05792
H	-1.94364	-2.15156	-1.35525	C	-3.56276	-0.44770	-0.96759
C	-2.58142	-0.48335	-0.22501	C	-4.61825	0.24204	-1.56449
C	2.40136	-3.01513	-0.85062	C	-4.93385	1.53274	-1.14313
C	2.83101	-0.16026	-1.85098	C	-4.19274	2.12694	-0.12049
C	3.60368	-0.93214	1.04843	C	-3.14377	1.43080	0.47819
H	1.70559	-3.20541	-1.67412	O	-0.45147	0.06191	0.33163
H	3.40519	-3.31083	-1.17523	H	3.63578	-2.08881	0.30285
H	2.11259	-3.65385	-0.00841	H	2.55616	-3.49259	0.39832
H	2.16981	-0.37925	-2.69835	H	3.39323	-3.12033	-1.11737
H	2.77859	0.91439	-1.64177	H	0.54052	-3.26648	-2.43814
H	3.85323	-0.39444	-2.16750	H	-0.27081	-3.43686	-0.86905
H	3.48339	-1.70426	1.81581	H	-0.71422	-2.11154	-1.96335
H	4.62385	-1.00416	0.65583	H	2.28151	-0.95494	-3.05616
H	3.49526	0.04333	1.53225	H	1.24378	0.31661	-2.39505
C	-3.40269	-0.09354	-1.29058	H	2.91171	0.14515	-1.81571
C	-2.68424	0.21384	0.98571	H	1.52641	-1.91738	2.27744
C	-4.29704	0.97020	-1.16280	H	-0.48430	-1.89312	3.66249
C	-4.38756	1.65694	0.04620	H	-2.61510	-1.38935	2.44434
C	-3.58092	1.27178	1.11813	H	-1.94208	0.22134	2.65219
H	-2.05422	-0.06970	1.82211	H	-3.31529	-1.45297	-1.29993
H	-3.64591	1.80321	2.06309	H	-5.19008	-0.22777	-2.35883
H	-5.08296	2.48359	0.15469	H	-5.75326	2.07287	-1.60712
H	-3.34875	-0.63859	-2.23100	H	-4.43649	3.13062	0.21453
H	-4.92613	1.25220	-2.00170	H	-2.58090	1.89812	1.28294
C	-0.08804	2.08005	-0.02709	Li	0.23947	1.84177	0.46083
H	-0.41963	2.15719	1.02067	C	2.14747	1.67758	1.60587
H	-0.98193	2.38892	-0.60582	C	3.47281	1.61624	0.84433
C	1.05886	3.06758	-0.27044	H	2.25621	1.24855	2.61321
H	0.76904	4.12078	-0.10655	H	1.88346	2.74018	1.77131
H	1.39293	3.02294	-1.32088	H	3.66003	0.57573	0.51882
C	2.26726	2.77322	0.61994	H	4.34663	1.89194	1.45690
H	2.58740	1.73792	0.45432	C	3.46513	2.51100	-0.39522
H	1.95452	2.82836	1.67216	H	2.59602	2.24969	-1.01638
C	3.44296	3.71672	0.37758	C	4.74155	2.41278	-1.22814
H	3.78824	3.64636	-0.66048	H	3.31268	3.55177	-0.07709
H	4.29187	3.48580	1.02873	H	4.90705	1.38503	-1.57143
H	3.15294	4.75754	0.55971	H	5.61444	2.70409	-0.63393
Li	-0.34222	0.61885	-1.63207	H	4.70499	3.05884	-2.11062
One imaginary frequency: -1398.12 cm^{-1}				One imaginary frequency: -1333.22 cm^{-1}			

Electronic Energy =-1075.25208555 Zero-point corrected electronic energy= -1074.828826 Zero-point corrected Gibbs free energy= -1074.858463				Electronic Energy = -1075.26388336 Zero-point corrected electronic energy=-1074.840053 Zero-point corrected Gibbs free energy=-1074.86895			
2a-TS- C^1				2b-TS- C^1			
C	-0.25747	1.12542	1.61226	C	-1.22182	-0.68687	1.91204
C	0.36206	2.32262	1.53247	C	-0.16995	-0.97635	2.70571
C	-0.57196	0.27515	0.47520	C	-1.14046	-0.33466	0.49660
H	-0.56252	0.74409	2.58806	H	-2.22648	-0.67451	2.33603
O	-0.18179	0.88302	-0.79695	O	0.24520	-0.37880	-0.01795
H	-1.91945	0.29227	0.21727	H	-1.32109	1.02639	0.31011
Si	-0.24802	-1.56664	0.64203	Si	-2.17112	-1.49758	-0.56875
C	0.84457	2.83938	0.20260	C	1.22002	-0.95680	2.13166
H	0.53522	2.92110	2.42243	H	-0.30852	-1.18725	3.76209
C	1.00194	1.69370	-0.79840	C	1.25458	-0.00582	0.93349
H	1.79883	3.37174	0.29907	H	1.54739	-1.95060	1.79270
H	0.13737	3.56389	-0.22521	H	1.95595	-0.61562	2.86975
H	1.03744	2.10688	-1.81322	H	1.03952	1.00996	1.30039
C	2.23546	0.81933	-0.63213	C	2.57810	-0.01807	0.21018
C	1.41084	-2.10798	1.36316	C	-1.33234	-3.18478	-0.68806
C	-0.47941	-2.34985	-1.06042	C	-2.36875	-0.83043	-2.33049
C	-1.59839	-2.19490	1.80756	C	-3.87342	-1.70563	0.21940
H	2.24194	-1.86890	0.69281	H	-0.36113	-3.09495	-1.18573
H	1.41389	-3.18888	1.54837	H	-1.94198	-3.89811	-1.25348
H	1.59269	-1.60042	2.31751	H	-1.16182	-3.59537	0.31327
H	0.35879	-2.09981	-1.71830	H	-1.40490	-0.81018	-2.85424
H	-1.40380	-1.99445	-1.53141	H	-2.78916	0.18189	-2.34358
H	-0.53930	-3.44080	-0.98288	H	-3.03613	-1.47980	-2.90697
H	-1.53461	-1.70393	2.78550	H	-3.80498	-2.32682	1.11858
H	-1.50670	-3.27462	1.96866	H	-4.55460	-2.20081	-0.48098
H	-2.59065	-1.98873	1.39215	H	-4.31907	-0.74719	0.50405
C	2.48925	-0.12709	-1.63225	C	3.50165	1.01403	0.38961
C	3.13617	0.92993	0.42834	C	2.91096	-1.09475	-0.61994
C	3.61327	-0.94633	-1.57988	C	4.74371	0.97158	-0.24602
C	4.51230	-0.82292	-0.51869	C	5.06846	-0.10352	-1.07195
C	4.26992	0.11558	0.48246	C	4.14809	-1.13708	-1.25845
H	2.95346	1.64706	1.22298	H	2.18949	-1.89479	-0.76220
H	4.96232	0.21373	1.31315	H	4.39758	-1.97755	-1.89905
H	5.39418	-1.45458	-0.47413	H	6.03355	-0.13792	-1.56801
H	1.79346	-0.21292	-2.46395	H	3.24848	1.85490	1.03145
H	3.79216	-1.67393	-2.36591	H	5.45462	1.77869	-0.09821
C	-3.38474	0.66617	-0.04586	C	-1.20118	2.54914	0.18557
H	-3.58380	0.29993	0.97617	H	-1.37406	2.63711	1.27196
C	-4.47729	0.07386	-0.94332	C	-2.45132	3.06779	-0.52582
H	-5.46531	0.51033	-0.69840	H	-2.60129	4.14785	-0.33575
H	-4.31977	0.34363	-2.00365	H	-2.32255	2.98857	-1.61880
C	-4.58591	-1.44687	-0.83123	C	-3.72223	2.31701	-0.12654
H	-3.63525	-1.93102	-1.08188	H	-3.65496	1.25949	-0.40054
H	-4.83432	-1.73392	0.19695	H	-3.87057	2.36247	0.95896

Li	-1.87445	0.88854	-1.62700
C	-3.47330	2.19615	-0.00103
H	-3.35069	2.65327	-0.99777
H	-2.69339	2.62042	0.64382
H	-4.44615	2.56821	0.36447
H	-5.35991	-1.85467	-1.48954

One imaginary frequency: -1338.39 cm^{-1}
Electronic Energy = -1075.25545837
Zero-point corrected electronic energy=-1074.832071
Zero-point corrected Gibbs free energy=-1074.860097

Li	-0.13116	1.15569	-1.14811
C	-0.00084	3.45082	-0.14601
H	0.24194	3.45913	-1.22226
H	0.91309	3.15741	0.38721
H	-0.18648	4.51030	0.10466
H	-4.61384	2.73311	-0.60679

One imaginary frequency: 1363.02 cm^{-1}
Electronic Energy = -1075.25261332
Zero-point corrected electronic energy=-1074.829315
Zero-point corrected Gibbs free energy=-1074.858073

16. Energies and Cartesian Coordinates for optimized geometries of Intermediates B, C, D, and products 3a and 4a of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism in Tetrahydrofuran solvent at 195 K

B			
C	-1.02622	2.05193	0.45743
C	0.04809	2.76347	0.85231
H	-1.96792	2.25474	0.97104
O	-0.58892	0.94503	-1.61090
Si	-2.21179	-0.61778	-0.06201
C	1.52611	2.65775	0.57016
H	-0.16595	3.51599	1.61432
C	2.10023	1.66794	-0.41261
H	1.84630	3.67526	0.30280
H	1.94923	2.51172	1.59015
H	3.03111	2.01592	-0.86923
C	2.12143	0.27590	-0.07782
C	-3.92571	-0.23889	-0.74594
C	-1.43630	-2.07201	-0.94935
C	-2.30410	-0.83324	1.80140
H	-3.88430	-0.06746	-1.82603
H	-4.59905	-1.08257	-0.56072
H	-4.35791	0.64837	-0.27244
H	-1.47073	-1.91370	-2.03147
H	-0.39002	-2.18941	-0.64792
H	-1.97368	-2.99769	-0.71919
H	-2.77367	0.03746	2.27060
H	-2.90522	-1.71414	2.05038
H	-1.31019	-0.96310	2.23850
C	2.89597	-0.65777	-0.83502
C	1.38316	-0.29077	1.00276
C	2.92600	-2.01022	-0.54473
C	2.18914	-2.53943	0.52926
C	1.43091	-1.65581	1.29354
H	0.79556	0.35747	1.64739

C			
O	-2.35522	0.68009	-1.08588
C	-1.26158	0.59381	-0.22501
C	-1.48486	1.50558	0.97914
C	-0.87902	2.68802	0.84391
C	-0.06609	2.75081	-0.42753
C	0.01285	1.26984	-0.87440
H	-0.10621	1.16617	-1.95726
C	1.32734	0.62913	-0.48355
C	1.96968	0.90800	0.73123
C	3.15533	0.26539	1.08258
C	3.72962	-0.67432	0.22535
C	3.11173	-0.95191	-0.99363
C	1.92900	-0.29971	-1.34113
Si	-1.17908	-1.26536	0.25056
C	-2.86508	-1.68544	1.00743
C	-0.96390	-2.35383	-1.27823
C	0.11233	-1.76613	1.54292
H	-2.16640	1.24604	1.78779
H	-0.97913	3.53227	1.52197
H	0.92727	3.18978	-0.28039
H	-0.57802	3.37165	-1.17399
H	1.52828	1.62619	1.41704
H	3.63004	0.49420	2.03263
H	4.65122	-1.17780	0.50118
H	3.55308	-1.67048	-1.67837
H	1.45890	-0.51321	-2.29853
H	-2.88495	-2.73671	1.31682
H	-3.67068	-1.53177	0.28281
H	-3.07797	-1.07467	1.89183
H	-1.26184	-3.38351	-1.04917

H	0.86003	-2.03348	2.14033
H	3.48754	-0.27816	-1.66760
H	3.53806	-2.66969	-1.15627
C	-1.12105	0.92424	-0.49435
Li	0.96881	1.77422	-2.25293
H	2.21492	-3.60002	0.75731

Electronic Energy = -916.924896330
Zero-point corrected electronic energy=-916.634549
Zero-point corrected Gibbs free energy=-916.660303

H	0.07483	-2.37324	-1.61974
H	-1.59186	-1.98817	-2.09672
H	-0.11830	-2.76720	1.92693
H	0.11063	-1.07108	2.39062
H	1.12449	-1.78083	1.12558
Li	-4.07951	0.81375	-1.19877

Electronic Energy = -916.975402983
Zero-point corrected electronic energy=-916.681238
Zero-point corrected Gibbs free energy=-916.706067

D

O	-1.50241	1.63464	-0.33166
C	-1.78598	0.34837	-0.23237
Si	-3.56386	-0.02428	0.30664
C	-3.92647	-1.87660	0.34769
C	-3.85654	0.70671	2.02312
C	-4.75527	0.80921	-0.89926
C	-0.90358	-0.65767	-0.49033
C	0.49314	-0.43481	-0.93054
C	1.23950	-1.49420	-1.68784
C	1.64677	-1.18474	-0.26847
H	1.34674	-1.91284	0.48133
C	2.92708	-0.49189	0.02737
C	3.48764	0.44323	-0.85595
C	4.68064	1.09357	-0.54954
C	5.34522	0.82316	0.64761
C	4.80082	-0.10615	1.53342
C	3.60555	-0.75435	1.22511
H	-4.96155	-2.05410	0.65981
H	-3.26829	-2.39640	1.05173
H	-3.79032	-2.32645	-0.64132
H	-4.90305	0.59325	2.32661
H	-3.61381	1.77432	2.02922
H	-3.22790	0.21274	2.77113
H	-5.79451	0.66989	-0.58205
H	-4.64745	0.39426	-1.90690
H	-4.55852	1.88495	-0.95163
H	-1.22982	-1.69104	-0.37817
H	0.72576	0.59608	-1.18800
H	0.72588	-2.43529	-1.86234
H	1.92378	-1.19530	-2.47712
H	2.98870	0.66823	-1.79550
H	5.09432	1.81315	-1.25009
H	6.27557	1.32935	0.88512
H	5.30699	-0.32864	2.46827
H	3.18860	-1.47645	1.92266
Li	-1.21966	3.26669	-0.84752

3a

O	0.91976	-0.84212	-0.98211
C	1.60170	0.01130	-0.43153
C	1.00887	1.35878	-0.05448
C	-0.47097	1.47423	-0.30894
H	-0.77451	1.29093	-1.33699
C	-1.43453	0.96811	0.73640
H	-0.97376	0.60919	1.65415
C	-2.66441	0.22479	0.34969
C	-3.42043	0.56529	-0.78043
C	-4.56202	-0.15790	-1.11964
C	-4.97301	-1.23690	-0.33576
C	-4.22924	-1.58467	0.79086
C	-3.08705	-0.85952	1.12752
C	-1.29259	2.45116	0.47246
Si	3.45185	-0.39640	-0.00424
C	4.14687	-1.37736	-1.44207
C	4.39757	1.20278	0.28233
C	3.39495	-1.43161	1.56451
H	1.57386	2.12645	-0.60518
H	1.23855	1.54154	1.00638
H	-3.11927	1.40220	-1.40605
H	-5.13234	0.12253	-2.00017
H	-5.86207	-1.79975	-0.60188
H	-4.53567	-2.42334	1.40882
H	-2.51088	-1.13860	2.00595
H	-0.79246	3.04609	1.23084
H	-2.11874	2.94891	-0.02591
H	4.17327	-0.77436	-2.35462
H	3.53099	-2.26097	-1.63336
H	5.16631	-1.70965	-1.22154
H	4.39415	1.83407	-0.61165
H	5.44002	0.98384	0.53612
H	3.96498	1.77610	1.10873
H	2.81010	-2.34219	1.40218
H	2.94242	-0.87420	2.39071
H	4.40678	-1.72305	1.86414

Electronic Energy = -916.970928990 Zero-point corrected electronic energy=-916.678708 Zero-point corrected Gibbs free energy=-916.706653	Electronic Energy = -909.976472118 Zero-point corrected electronic energy=-909.673027 Zero-point corrected Gibbs free energy=-909.700434
4a O 2.36278 0.71978 1.21369 C 1.26959 0.63116 0.26639 Si 1.32706 -1.23519 -0.21421 C 3.04483 -1.50485 -0.94472 C 1.14676 -2.29707 1.32818 C 0.06021 -1.72715 -1.51618 C 1.54992 1.57511 -0.88618 C 0.90274 2.73552 -0.74374 C 0.02244 2.74480 0.48197 C -0.02190 1.25240 0.90160 H 0.06483 1.13337 1.98612 C -1.30380 0.57368 0.46136 C -1.90558 0.84335 -0.77450 C -3.06129 0.17210 -1.16866 C -3.64059 -0.78356 -0.33300 C -3.06140 -1.05004 0.90684 C -1.90783 -0.37064 1.29787 H 2.64086 1.64450 1.27504 H 3.21298 -2.57390 -1.11486 H 3.82086 -1.13745 -0.26716 H 3.15721 -0.99472 -1.90722 H 1.39013 -3.33792 1.08813 H 0.12784 -2.27304 1.72379 H 1.83250 -1.95694 2.11012 H 0.35908 -2.68752 -1.95205 H 0.01415 -0.98967 -2.32485 H -0.94504 -1.83485 -1.09765 H 2.27157 1.35043 -1.66686 H 1.00799 3.59467 -1.40015 H -0.97771 3.14337 0.28420 H 0.46193 3.37961 1.26214 H -1.45979 1.57554 -1.44286 H -3.50817 0.39128 -2.13398 H -3.50973 -1.78005 1.57421 H -1.46809 -0.57259 2.27177 H -4.53924 -1.30854 -0.64192 Electronic Energy = -909.988378636 Zero-point corrected electronic energy=-909.683868 Zero-point corrected Gibbs free energy=-909.708472	

17. Energies and Cartesian Coordinates for optimized geometries of transition states TS-Bs, TS-C and TS- D of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism in Tetrahydrofuran solvent at 195 K

TS-Bs

C	1.05996	1.75961	-1.09370
C	0.06822	2.69604	-1.21840
C	1.17653	0.93687	0.06457
H	1.70855	1.55470	-1.94633
O	0.51564	1.36298	1.12310
Si	1.93675	-0.77774	0.07183
C	-1.09838	2.84698	-0.26939
H	-0.01026	3.25078	-2.15127
C	-1.41385	1.69712	0.64270
H	-0.99646	3.75495	0.34119
H	-1.98861	3.02095	-0.89658
H	-1.79217	1.98035	1.62376
C	-1.81055	0.39698	0.21276
C	3.68031	-0.71878	0.82296
C	0.90873	-1.93588	1.14607
C	2.11802	-1.47427	-1.67462
H	3.65249	-0.32817	1.84663
H	4.13141	-1.71751	0.85659
H	4.33747	-0.06875	0.23472
H	1.40629	-2.90651	1.25300
H	0.77535	-1.51239	2.14747
H	-0.08399	-2.09138	0.71159
H	2.73046	-0.81663	-2.30113
H	2.60052	-2.45805	-1.65117
H	1.13624	-1.57954	-2.14731
C	-2.53524	-0.44935	1.10073
C	-1.45128	-0.15172	-1.04503
C	-2.90631	-1.73169	0.74850
C	-2.56278	-2.24984	-0.51606
C	-1.84850	-1.44957	-1.39686
H	-0.91873	0.45378	-1.76608
H	-1.57773	-1.83566	-2.37697
H	-2.85223	-3.25869	-0.79381
H	-2.81410	-0.05791	2.07772
H	-3.46879	-2.34216	1.44996
Li	0.82514	1.96907	2.78406

One imaginary frequency: -340.80 cm^{-1}
Electronic Energy = -916.903458330
Zero-point corrected electronic energy=-916.612968
Zero-point corrected Gibbs free energy=-916.637858

TS-C

C	1.60530	1.87574	-0.78659
C	0.69456	2.83951	-0.59532
C	1.72971	0.74975	0.22486
H	2.36203	1.94055	-1.56852
O	2.46506	0.99079	1.22588
Si	1.68589	-1.12206	-0.19842
C	-0.24340	2.67864	0.58591
H	0.65946	3.73193	-1.21889
C	-0.36757	1.20943	0.95145
H	0.18382	3.24599	1.42263
H	-1.21257	3.14967	0.37606
H	-0.00425	0.92825	1.93556
C	-1.56031	0.49152	0.55393
C	1.34268	-2.06342	1.39360
C	0.40483	-1.60900	-1.52135
C	3.37900	-1.57012	-0.89120
H	0.43687	-2.67109	1.30985
H	2.17967	-2.72533	1.63555
H	1.21755	-1.36016	2.22229
H	-0.64457	-1.49893	-1.21428
H	0.56812	-1.14581	-2.50277
H	0.54152	-2.68346	-1.68792
H	4.16108	-1.31028	-0.17119
H	3.44040	-2.64566	-1.09002
H	3.58406	-1.03834	-1.82613
C	-1.89677	-0.74605	1.17618
C	-2.40392	0.89169	-0.51973
C	-2.93885	-1.53398	0.72639
C	-3.72432	-1.14060	-0.37224
C	-3.45135	0.08016	-0.97544
H	-2.26632	1.86650	-0.98928
H	-4.06431	0.42663	-1.80332
H	-4.53738	-1.76597	-0.72454
H	-1.30763	-1.06791	2.03095
H	-3.15440	-2.47031	1.23439
Li	-0.29452	0.65224	-1.36745

One imaginary frequency: -149.51 cm^{-1}
Electronic Energy = -916.898687869
Zero-point corrected electronic energy=-916.607183
Zero-point corrected Gibbs free energy=-916.632386

TS-D

C	-1.03603	-0.90991	-0.45386
C	0.21697	-1.15405	0.06049
C	-1.92065	0.14205	0.00308
H	-1.37253	-1.50896	-1.29719
O	-1.43222	1.18738	0.50596
Si	-3.83993	0.02208	-0.16512
C	0.84059	-0.59632	1.29415
H	0.82924	-1.87342	-0.48518
C	1.69232	0.48959	0.67314
H	0.09270	-0.17719	1.96971
H	1.41527	-1.36194	1.83431
H	1.45907	1.50188	1.00919
C	3.04689	0.25757	0.26707
C	-4.46870	-0.50695	1.52562
C	-4.47015	1.73218	-0.61000
C	-4.28620	-1.24920	-1.47455
H	-4.15940	0.20845	2.29378
H	-5.56235	-0.55805	1.52547
H	-4.08015	-1.49334	1.79699
H	-4.12230	2.46500	0.12419
H	-4.11543	2.04151	-1.59791
H	-5.56462	1.74879	-0.62016
H	-3.89960	-2.23942	-1.21330
H	-5.37464	-1.32778	-1.56586
H	-3.88598	-0.97089	-2.45474
C	3.90798	1.34630	-0.05325
C	3.62553	-1.03635	0.15536
C	5.22094	1.15698	-0.45524
C	5.76380	-0.13069	-0.56588
C	4.94493	-1.21701	-0.25157
H	3.02780	-1.91421	0.38768
H	5.34012	-2.22783	-0.32245
H	6.79063	-0.27818	-0.88380
H	3.51504	2.35821	0.03028
H	5.83548	2.02451	-0.68439
Li	0.19302	1.27651	-0.75664

One imaginary frequency: -273.00 cm^{-1}
Electronic Energy = -916.914972843
Zero-point corrected electronic energy=-916.625058
Zero-point corrected Gibbs free energy=-916.651807

18. Energies and Cartesian coordinates of optimized geometries for stationary points of the 2-silyl-6-aryl-5,6-dihydro-(2H)-pyran mechanism with two molecules of dimethyl ether obtained at 195 K in Tetrahydrofuran solvent

A				A’			
C	0.38129	0.64422	2.49072	C	0.50079	-0.99586	1.98577
C	1.31599	-0.21439	1.92339	C	0.32336	0.30809	1.53957
H	0.62992	1.17483	3.40406	H	0.76181	-1.17637	3.02407
C	-1.08243	0.53203	2.10673	C	-0.03967	-2.16117	1.17439
C	1.08596	-0.92771	0.74147	C	0.01659	0.62494	0.21233
H	2.30338	-0.30553	2.37837	H	0.48327	1.13799	2.22895
O	-0.20203	-0.61492	0.16781	O	-0.03599	-0.54128	-0.63287
C	-1.26019	-0.64180	1.14024	C	-0.77216	-1.66281	-0.07904
H	-1.48907	1.44436	1.64026	H	-0.73798	-2.76769	1.77065
H	-1.70182	0.34675	2.99744	H	0.75016	-2.85677	0.85053
H	-1.14568	-1.58119	1.70427	H	-0.71411	-2.42315	-0.86567
Li	0.86318	1.11402	0.18044	Li	1.86486	-0.42968	0.18034
O	2.46568	2.05113	-0.40408	O	3.49366	0.55595	0.60907
O	-0.36001	2.46191	-0.49063	O	2.75682	-1.79437	-0.86592
C	-0.29600	3.73797	0.12345	C	3.80982	-2.52103	-0.25142
H	-0.43482	4.52849	-0.62429	H	4.54550	-2.83220	-1.00271
H	0.69298	3.82809	0.57691	H	4.27741	-1.85311	0.47276
H	-1.06801	3.82992	0.89796	H	3.41358	-3.40868	0.25809
C	2.56386	2.72582	-1.64813	C	3.98827	1.28068	-0.50658
H	1.54716	2.91979	-1.99079	H	3.90089	0.62889	-1.37776
H	3.09088	2.10155	-2.38073	H	3.39631	2.19214	-0.66361
H	3.10398	3.67230	-1.52416	H	5.03914	1.55112	-0.34952
C	3.73588	1.71775	0.13104	C	3.54890	1.30927	1.81004
H	4.26844	1.03372	-0.54264	H	2.93391	2.21444	1.72382
H	3.56549	1.22808	1.09026	H	3.15427	0.67618	2.60561
H	4.33514	2.62452	0.27686	H	4.58534	1.59007	2.03172
C	-1.59395	2.22727	-1.15078	C	2.07276	-2.55221	-1.85161
H	-2.42888	2.29739	-0.44154	H	1.63539	-3.45561	-1.40555
H	-1.73408	2.95798	-1.95658	H	2.76442	-2.84374	-2.65083
H	-1.55826	1.21614	-1.55823	H	1.28039	-1.91864	-2.25070
Si	2.14123	-2.06083	-0.23175	Si	-0.54971	2.20414	-0.53518
C	3.80849	-2.23634	0.63912	C	-2.43359	2.37113	-0.63287
H	3.68989	-2.70019	1.62382	H	-2.73513	3.25142	-1.21325
H	4.47887	-2.86809	0.04618	H	-2.87071	1.47977	-1.09818
H	4.29594	-1.26536	0.77659	H	-2.86021	2.45444	0.37274
C	1.36722	-3.77664	-0.44552	C	0.10676	2.34168	-2.30374
H	1.96806	-4.40862	-1.10966	H	-0.26308	3.24768	-2.79664
H	0.36451	-3.69048	-0.87942	H	1.20200	2.36540	-2.31524
H	1.27180	-4.28251	0.52097	H	-0.21631	1.47856	-2.89594
C	2.41895	-1.39049	-1.98481	C	0.11922	3.63951	0.49779
H	1.45543	-1.22510	-2.48161	H	1.21294	3.68120	0.45480
H	3.00160	-2.08398	-2.60204	H	-0.27034	4.59227	0.12239
H	2.94627	-0.42998	-1.95226	H	-0.17730	3.54957	1.54844
C	-2.57819	-0.67519	0.39540	C	-2.23153	-1.30309	0.09423
C	-3.72834	-0.06952	0.90998	C	-3.09421	-1.45829	-0.99656
C	-2.66539	-1.35016	-0.82755	C	-2.74454	-0.77550	1.28380
C	-4.93804	-0.13259	0.21646	C	-4.43755	-1.09723	-0.90813
H	-3.68559	0.46305	1.85562	H	-2.70482	-1.86623	-1.92707
C	-3.87091	-1.41141	-1.52383	C	-4.08907	-0.41640	1.37806

H	-1.77243	-1.81331	-1.23565	H	-2.08375	-0.65104	2.13714
C	-5.01323	-0.80070	-1.00443	C	-4.93888	-0.57250	0.28367
H	-5.82092	0.34500	0.63094	H	-5.09210	-1.22751	-1.76496
H	-3.91887	-1.93546	-2.47395	H	-4.47266	-0.00761	2.30851
H	-5.95299	-0.84631	-1.54626	H	-5.98459	-0.28932	0.35843
Electronic Energy = -1226.89180722 Zero-point corrected electronic energy=-1226.432274 Zero-point corrected Gibbs free energy=-1226.465492				Electronic Energy = -1226.891071 Zero-point corrected electronic energy=-1226.431469 Zero-point corrected Gibbs free energy = -1226.464018			
TS-B				TS-B'			
C	1.43420	-3.04214	1.27799	C	0.51689	-0.79046	2.13269
C	2.28118	-2.04702	0.85205	C	0.23797	0.46323	1.63096
H	1.87976	-3.96000	1.65710	H	0.69904	-0.87622	3.20180
C	-0.05331	-3.08998	1.04625	C	0.23787	-2.11614	1.42955
C	1.80245	-0.83997	0.27130	C	-0.01752	0.66477	0.23659
H	3.35736	-2.21473	0.89229	H	0.15781	1.30779	2.31548
O	0.51488	-0.64044	0.37756	O	0.37417	-0.30549	-0.54006
C	-0.55398	-2.30749	-0.12352	C	-0.63258	-2.12308	0.22118
H	-0.30622	-4.14713	0.86245	H	-0.25574	-2.72440	2.20635
H	-0.61717	-2.82311	1.95038	H	1.16917	-2.65709	1.20403
Li	-0.77099	0.61411	0.69920	H	-0.33266	-2.78614	-0.58526
O	-0.00985	1.78148	2.01016	Li	2.02165	-0.45954	0.39081
O	-1.41697	1.67862	-0.74598	O	3.34505	0.95301	0.42825
C	-2.46789	2.62972	-0.75360	O	3.05351	-1.72914	-0.56989
H	-2.10310	3.59733	-1.12069	C	4.37230	-2.13270	-0.24094
H	-2.82894	2.73203	0.27141	H	5.00990	-2.10698	-1.13274
H	-3.28957	2.27754	-1.38783	H	4.75084	-1.42701	0.49964
C	0.02742	3.19692	1.94287	H	4.37019	-3.14731	0.17488
H	-0.72806	3.51269	1.22219	C	3.66365	1.41621	-0.87765
H	1.01343	3.53760	1.60531	H	3.70483	0.54112	-1.52801
H	-0.19171	3.63075	2.92564	H	2.89067	2.10729	-1.23546
C	1.01832	1.24742	2.83377	H	4.63514	1.92397	-0.87135
H	2.00177	1.51182	2.42517	C	3.22572	2.01867	1.35934
H	0.91186	0.16193	2.82542	H	2.39253	2.67710	1.08163
H	0.92217	1.63635	3.85434	H	3.02835	1.57782	2.33705
C	-0.92927	1.38976	-2.04791	H	4.15697	2.59588	1.39255
H	-1.75517	1.08403	-2.69992	C	2.45383	-2.53316	-1.57570
H	-0.42383	2.26818	-2.46889	H	2.32954	-3.56278	-1.21704
H	-0.22246	0.56402	-1.94378	H	3.07758	-2.53452	-2.47735
Si	2.80658	0.23192	-0.89358	H	1.48062	-2.09111	-1.79169
C	2.58942	-0.28987	-2.70238	Si	-0.97440	2.12320	-0.48585
H	3.09098	0.41373	-3.37683	C	-2.21966	1.49675	-1.74563
H	1.53574	-0.34511	-2.99370	H	-2.67051	2.33401	-2.29047
H	3.02789	-1.28178	-2.85572	H	-1.72421	0.84260	-2.47054
C	2.25160	2.02781	-0.68171	H	-3.01302	0.92103	-1.26013
H	2.48838	2.63775	-1.56029	C	0.21242	3.28624	-1.39476
H	2.75692	2.47093	0.18421	H	-0.33998	4.11401	-1.85452
H	1.17208	2.08581	-0.50074	H	0.96018	3.71559	-0.71897

C	4.64040	0.09602	-0.46717	H	0.73833	2.74961	-2.19222
H	5.22557	0.78954	-1.08105	C	-1.81328	3.09921	0.89308
H	5.02031	-0.91458	-0.64922	H	-2.35564	3.95875	0.48416
H	4.81898	0.34270	0.58497	H	-2.52469	2.46601	1.43337
H	-0.09348	-2.53519	-1.08423	H	-1.07853	3.47913	1.61183
C	-1.83428	-1.68179	-0.15987	C	-1.97141	-1.66241	0.17152
C	-2.45879	-1.17521	1.01460	C	-2.79900	-2.03152	-0.93291
C	-2.50815	-1.44339	-1.39117	C	-2.55734	-0.80932	1.14612
C	-3.67273	-0.48563	0.94978	C	-4.11418	-1.62931	-1.02841
H	-1.98737	-1.32104	1.98332	H	-2.37122	-2.66606	-1.70675
C	-3.71075	-0.76345	-1.44054	C	-3.89977	-0.41880	1.04276
H	-2.05631	-1.81225	-2.30981	H	-1.98994	-0.51181	2.01787
C	-4.31213	-0.27097	-0.26840	C	-4.68622	-0.81280	-0.03091
H	-4.11742	-0.11126	1.86873	H	-4.71244	-1.94322	-1.87970
H	-4.19497	-0.60679	-2.40157	H	-4.32494	0.21277	1.81945
H	-5.25335	0.26737	-0.31404	H	-5.72160	-0.49524	-0.10618
One imaginary frequency: -342.04 cm^{-1} Electronic Energy = -1226.853739 Zero-point corrected electronic energy=-1226.397764 Zero-point corrected Gibbs free energy=-1226.429974				One imaginary frequency: -173.70 cm^{-1} Electronic Energy = -1226.859165 Zero-point corrected electronic energy=-1226.402329 Zero-point corrected Gibbs free energy=-1226.43396			
B				TS-C			
C	0.57776	-1.97513	1.24099	C	3.30957	-1.88925	1.13475
C	-0.11039	-1.60919	2.34096	C	3.36039	-0.56293	1.24285
H	1.16958	-2.88997	1.31935	H	3.63349	-2.55801	1.93179
O	-0.11053	-0.75688	-0.70074	C	2.83260	-2.43926	-0.18838
Si	2.58071	-1.22177	-0.80677	C	3.01331	0.31438	0.06294
C	-0.86602	-0.36388	2.73686	H	3.73445	-0.06058	2.13618
H	-0.02956	-2.31414	3.17200	O	3.95981	0.64559	-0.71564
C	-1.19060	0.73725	1.76357	C	1.99418	-1.41392	-0.93426
H	-1.79078	-0.72330	3.20950	H	2.27930	-3.37644	-0.03082
H	-0.26716	0.01303	3.59764	H	3.71289	-2.71550	-0.78488
H	-2.17240	1.19357	1.91447	H	2.38351	-1.09130	-1.89784
C	-0.17902	1.63431	1.32441	Li	-1.62849	-0.18958	-0.05370
C	2.77836	-2.83086	-1.76769	O	-2.78495	-0.19159	1.49733
C	2.60707	0.26061	-1.95071	O	-2.26487	1.50502	-0.76207
C	3.86251	-1.14303	0.56331	C	-2.39303	1.84704	-2.13759
H	2.00202	-2.92824	-2.53284	H	-1.91977	2.81578	-2.33143
H	3.75265	-2.85394	-2.26747	H	-1.89031	1.07702	-2.72145
H	2.71960	-3.69992	-1.10453	H	-3.45292	1.89372	-2.41322
H	1.91779	0.10171	-2.78602	C	-2.48550	-0.75368	2.76814
H	2.29805	1.16286	-1.41138	H	-1.41307	-0.64466	2.93199
H	3.61018	0.42093	-2.35890	H	-3.03456	-0.22022	3.55193
H	3.81202	-2.03731	1.19281	H	-2.75829	-1.81543	2.79051
H	4.86905	-1.08852	0.13518	C	-4.16539	-0.30027	1.17423
H	3.71383	-0.26700	1.20068	H	-4.76951	0.23086	1.91880
C	-0.49889	2.84029	0.62191	H	-4.30900	0.15395	0.19152
C	1.21804	1.40544	1.52374	H	-4.46685	-1.35414	1.13979

C	0.47156	3.70731	0.15387	C	-2.75138	2.54733	0.07679
C	1.83937	3.45090	0.35658	H	-3.77865	2.80833	-0.20442
C	2.18503	2.29401	1.05521	H	-2.11125	3.43274	-0.01774
H	1.53647	0.52683	2.08024	H	-2.73666	2.18055	1.10325
H	3.23576	2.07525	1.24020	Si	1.63697	1.61328	0.27365
H	-1.55069	3.06882	0.44897	C	0.93367	2.10623	-1.39698
H	0.16594	4.60599	-0.37895	H	0.28566	2.98441	-1.29584
C	0.80009	-1.26884	-0.04306	H	1.76153	2.36659	-2.06495
Li	-1.75774	-0.08632	-0.12384	H	0.35835	1.30235	-1.86112
H	2.59793	4.13330	-0.01255	C	2.42917	3.15632	1.02614
O	-3.01118	-1.55855	-0.09323	H	3.20057	3.55013	0.35665
C	-3.51331	-2.01106	1.15403	H	1.68088	3.94120	1.18500
O	-2.29380	0.96363	-1.62572	H	2.89761	2.93365	1.99084
C	-1.36899	1.65293	-2.45364	C	0.32740	0.98462	1.48399
H	-1.66869	1.56174	-3.50509	H	0.15947	-0.08786	1.33622
H	-0.39270	1.19243	-2.29495	H	0.68381	1.10250	2.51336
H	-1.32063	2.71124	-2.17236	H	-0.62121	1.52718	1.40419
C	-3.58455	1.54659	-1.63662	C	0.57897	-1.63246	-0.93850
H	-4.22135	0.93640	-0.99383	C	-0.10758	-2.29717	0.12955
H	-3.99253	1.55554	-2.65463	C	-0.25168	-1.23645	-2.03232
H	-3.54503	2.57402	-1.25312	C	-1.46126	-2.61066	0.06060
H	-2.74365	-2.57834	1.69369	H	0.45355	-2.58462	1.01538
H	-4.39543	-2.64418	1.00033	C	-1.60589	-1.54925	-2.09084
H	-3.78921	-1.12837	1.73286	H	0.21236	-0.72980	-2.87544
C	-2.61512	-2.62994	-0.93608	C	-2.23909	-2.24668	-1.04890
H	-2.24249	-2.19278	-1.86319	H	-1.92592	-3.13353	0.89272
H	-3.47148	-3.28069	-1.14922	H	-2.18035	-1.26206	-2.96774
H	-1.81714	-3.21509	-0.46090	H	-3.29193	-2.49978	-1.10344
Electronic Energy = -1226.877397 Zero-point corrected electronic energy=-1226.420906 Zero-point corrected Gibbs free energy=-1226.453776				One imaginary frequency: -219.26 Electronic Energy = -1226.85845839 Zero-point corrected electronic energy=-1226.400434 Zero-point corrected Gibbs free energy=-1226.430819			
TS-D				C			
C	-0.14955	-2.07868	-0.40995	C	-0.67150	-0.78272	-1.65656
C	1.06281	-1.70385	0.11353	C	-0.40007	0.45175	-1.21659
H	-0.77526	-2.68932	0.24335	H	-1.20892	-1.02820	-2.57025
C	-0.74491	-1.77478	-1.74567	C	-0.16056	-1.83657	-0.70047
C	1.94889	-0.71491	-0.45159	C	0.19173	0.44226	0.19576
H	1.34770	-2.10928	1.08298	H	-0.69512	1.37287	-1.71806
O	1.51461	0.13766	-1.27132	O	-0.85798	0.61493	1.10664
C	-1.58025	-0.56050	-1.41555	C	0.75014	-1.03726	0.26776
H	-1.32405	-2.63068	-2.12193	H	0.38609	-2.63702	-1.21188
H	0.02434	-1.52453	-2.47833	H	-1.00064	-2.31020	-0.17655
H	-1.31129	0.36288	-1.93148	H	0.61995	-1.36331	1.30508
Li	-0.16389	0.65959	-0.25534	Li	-2.42407	0.21135	0.33519
O	-0.40168	0.69444	1.64584	O	-3.95512	0.67429	-0.77914
O	-0.09323	2.55301	-0.51095	O	-3.12212	-1.47253	0.95730

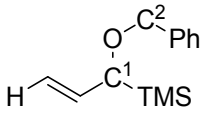
C	0.45144	3.10089	-1.70363	C	-4.10185	-2.32932	0.40127
H	1.02794	4.00466	-1.47325	H	-4.89898	-2.52615	1.12915
H	1.10502	2.34185	-2.13327	H	-4.51492	-1.82549	-0.47415
H	-0.35185	3.35210	-2.40704	H	-3.64708	-3.28076	0.09768
C	0.70977	1.16951	2.38586	C	-5.17627	0.88487	-0.08518
H	0.37939	1.61396	3.33225	H	-5.09948	0.36753	0.87291
H	1.40984	0.34809	2.59527	H	-5.34230	1.95510	0.08413
H	1.20262	1.92884	1.77373	H	-6.01456	0.47222	-0.65964
C	-1.15879	-0.28079	2.34833	C	-3.94053	1.30867	-2.04852
H	-0.53418	-1.15309	2.57933	H	-4.01229	2.39691	-1.93521
H	-1.98669	-0.57857	1.70146	H	-2.99867	1.04969	-2.53248
H	-1.54587	0.14802	3.28007	H	-4.77771	0.95023	-2.65888
C	-0.94391	3.46224	0.17000	C	-2.47251	-2.02490	2.09421
H	-1.32929	2.94491	1.04943	H	-2.03530	-3.00066	1.84480
H	-1.77595	3.76611	-0.47685	H	-3.18762	-2.15014	2.91627
H	-0.37865	4.35140	0.47379	H	-1.68269	-1.32084	2.36433
Si	3.80337	-0.56550	0.05619	Si	1.37984	1.90995	0.52684
C	4.11378	1.24436	0.45619	C	1.98108	1.89092	2.31647
H	5.18675	1.46054	0.47317	H	2.46686	2.84289	2.55946
H	3.64704	1.87638	-0.30665	H	1.13620	1.75140	2.99748
H	3.69840	1.51683	1.43125	H	2.70515	1.08958	2.49176
C	4.79552	-1.08543	-1.45405	C	0.35058	3.47678	0.27240
H	5.86768	-0.97622	-1.26102	H	0.93209	4.36499	0.54432
H	4.59878	-2.13029	-1.71284	H	0.04210	3.58940	-0.77340
H	4.53709	-0.46332	-2.31643	H	-0.54960	3.44490	0.89263
C	4.17832	-1.68187	1.52193	C	2.87944	2.06616	-0.62101
H	5.23853	-1.61327	1.78721	H	3.31771	3.06671	-0.52313
H	3.59373	-1.39957	2.40376	H	3.65352	1.32627	-0.39208
H	3.95807	-2.72791	1.28561	H	2.58551	1.92670	-1.66784
C	-2.85922	-0.61591	-0.80014	C	2.21418	-1.17060	-0.08969
C	-3.61775	0.57463	-0.58061	C	3.17736	-1.25196	0.92373
C	-3.46747	-1.82091	-0.33887	C	2.66071	-1.18668	-1.41853
C	-4.84931	0.55994	0.05420	C	4.53892	-1.32182	0.62826
H	-3.20162	1.52084	-0.92439	H	2.85122	-1.26013	1.96144
C	-4.70423	-1.82189	0.29746	C	4.01900	-1.26059	-1.72121
H	-2.95255	-2.76803	-0.48119	H	1.93749	-1.12603	-2.22755
C	-5.41656	-0.63841	0.51251	C	4.96675	-1.32227	-0.69904
H	-5.38088	1.49830	0.19672	H	5.26383	-1.38304	1.43501
H	-5.12102	-2.76936	0.63248	H	4.33938	-1.26506	-2.75925
H	-6.37850	-0.64667	1.01401	H	6.02525	-1.37758	-0.93435
One imaginary frequency: -245.28 Electronic Energy = -1226.87235897 Zero-point corrected electronic energy=-1226.416331 Zero-point corrected Gibbs free energy=-1226.449372				Electronic Energy = -1226.92262643 Zero-point corrected electronic energy=-1226.463551 Zero-point corrected Gibbs free energy=-1226.496865			
D							
C	-1.29890	-0.82425	-0.88842				
C	0.10683	-0.45363	-1.17758				

C	-2.05792	-0.26702	0.10156
H	-1.74030	-1.59593	-1.51857
O	-1.65119	0.66827	0.93799
Si	-3.86673	-0.77480	0.34518
C	0.69603	-0.65834	-2.54464
H	0.48624	0.40667	-0.62728
C	1.16385	-1.53293	-1.40891
H	0.05851	-1.12028	-3.29321
H	1.39996	0.07101	-2.93775
H	0.78377	-2.55152	-1.40402
C	2.50994	-1.37423	-0.80476
C	-4.11776	-1.36801	2.11946
C	-4.94697	0.74871	0.06759
C	-4.41064	-2.13946	-0.84240
H	-3.78724	-0.60246	2.82871
H	-5.17429	-1.58159	2.31529
H	-3.54367	-2.28022	2.31311
H	-4.62501	1.56214	0.72585
H	-4.86959	1.09803	-0.96776
H	-6.00052	0.53469	0.27789
H	-3.81054	-3.04599	-0.70999
H	-5.45935	-2.40062	-0.66155
H	-4.31839	-1.81948	-1.88561
C	3.11029	-2.45397	-0.14342
C	3.18948	-0.14759	-0.81559
C	4.33962	-2.31172	0.49933
C	4.99959	-1.08311	0.49029
C	4.41834	-0.00272	-0.17607
H	2.74864	0.71172	-1.31395
H	4.92422	0.95871	-0.19689
H	5.95672	-0.96910	0.98945
H	2.59876	-3.41310	-0.12341
H	4.78149	-3.16304	1.00882
Li	-0.38670	1.90156	1.06402
O	1.30700	1.27535	1.71493
O	-0.16870	2.84448	-0.61274
C	1.35177	-0.09279	2.11163
H	0.55039	-0.60732	1.57781
H	1.19216	-0.17262	3.19405
H	2.32324	-0.52631	1.84564
C	2.36257	2.03048	2.28493
H	2.24019	3.06744	1.96730
H	3.32987	1.64772	1.93746
H	2.32333	1.97916	3.37992
C	-1.23775	2.66862	-1.53618
H	-0.99244	1.86573	-2.24237
H	-1.42217	3.60340	-2.07888
H	-2.11576	2.37706	-0.95894
C	1.05863	3.12953	-1.25826
H	1.84275	3.12845	-0.49854
H	1.01729	4.10940	-1.74878

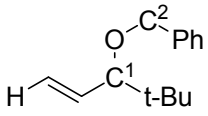
H 1.27732 2.36054 -2.01110 Electronic Energy = -1226.92768 Zero-point corrected electronic energy=-1226.469358 Zero-point corrected Gibbs free energy=-1226.50289	

19. Energies and Cartesian coordinates for optimized geometries of Reactants, Lithiated Intermediates and Anionic Intermediates of Structures 3a to 6b at 298.15 K

Numbering system followed for structures 3a and 3aC



3a



3aC

Silicon Analogues				Carbon Analogues			
3a_Reactant				3aC_Reactant			
C	3.21550	2.57739	0.46132	C	2.58276	2.70223	0.25315
C	2.20848	1.76585	0.78774	C	2.06480	1.54985	0.67346
C	1.48053	0.87568	-0.16936	C	1.67282	0.41715	-0.24063
Si	2.22728	-0.89499	-0.17841	C	2.48593	-1.41579	1.30778
C	2.27954	-1.47919	1.60748	C	2.06289	-1.88767	-1.11534
C	1.08335	-2.00443	-1.18103	C	4.01084	-0.47034	-0.44736
C	3.95230	-0.84634	-0.92579	O	0.33711	0.01518	0.02294
O	0.11535	0.73999	0.26040	H	2.86046	3.49078	0.94548
H	3.74643	3.15135	1.21321	H	2.75285	2.88962	-0.80529
H	3.54131	2.69037	-0.57065	H	1.88477	1.38349	1.73569
H	1.89378	1.67213	1.82710	H	1.74332	0.77004	-1.28626
H	1.52116	1.31754	-1.17711	H	1.44933	-1.62745	1.58598
H	1.29171	-1.36694	2.06635	H	2.90988	-0.72579	2.04457
H	2.99745	-0.89814	2.19488	H	3.05660	-2.34906	1.36159
H	2.56556	-2.53402	1.66960	H	1.03433	-2.18403	-0.89508
H	0.06257	-1.96066	-0.78478	H	2.69898	-2.77841	-1.07822
H	1.41766	-3.04609	-1.13028	H	2.09333	-1.49381	-2.13816
H	1.05638	-1.71469	-2.23673	H	4.42245	0.24312	0.27231
H	4.60331	-0.17625	-0.35516	H	4.08387	-0.02375	-1.44638
H	3.92826	-0.49562	-1.96294	H	4.63672	-1.36866	-0.43503
H	4.40593	-1.84293	-0.92071	C	-0.63500	0.96816	-0.33514
C	-0.82467	0.87115	-0.77814	H	-0.50040	1.25540	-1.39184
H	-0.52502	0.25483	-1.64193	H	-0.52257	1.88309	0.26580
H	-0.86754	1.91725	-1.12153	C	-2.01623	0.39201	-0.13833
C	-2.18655	0.42513	-0.30560	C	-2.20895	-0.93548	0.24223
C	-3.31157	0.72563	-1.07885	C	-3.13021	1.20818	-0.35489
C	-2.34440	-0.30573	0.87176	C	-3.50078	-1.43920	0.40062
C	-4.57589	0.29644	-0.68631	H	-1.34354	-1.56591	0.41609
H	-3.19640	1.30280	-1.99410	C	-4.41844	0.70546	-0.19965

C	-3.61245	-0.73334	1.26716	H	-2.98619	2.24625	-0.64806
H	-1.47042	-0.52570	1.47552	C	-4.60742	-0.62409	0.17969
C	-4.72987	-0.43618	0.49106	H	-3.64022	-2.47402	0.69885
H	-5.44183	0.53887	-1.29473	H	-5.27454	1.35048	-0.37299
H	-3.72544	-1.29789	2.18791	H	-5.61087	-1.01930	0.30318
H	-5.71535	-0.76848	0.80205	C	2.56274	-0.84106	-0.11156
Electronic Energy = -871.865971882 Zero-point corrected electronic energy=-871.568849 Zero-point corrected Gibbs free energy=-871.617773				Electronic Energy = -620.481917839 Zero-point corrected electronic energy=-620.172844 Zero-point corrected Gibbs free energy=-620.172844			
Lithiated Intermediates							
3aA-C[1]Li				3aCA-C[1]Li			
C	3.23047	2.33908	0.46287	C	-3.54138	1.94075	-0.77258
C	1.89929	1.93892	0.62442	C	-2.20245	1.50158	-0.79882
C	1.33097	0.71787	0.24088	C	-1.59452	0.41588	-0.17155
Si	2.27669	-0.86400	-0.04898	C	-2.93272	-1.53756	-1.02169
C	3.37045	-1.37565	1.39708	C	-1.29356	-1.88053	0.83423
C	1.06141	-2.22920	-0.48676	C	-3.39703	-0.66719	1.28715
C	3.44316	-0.63801	-1.56138	O	-0.22435	0.26270	-0.45628
O	-0.04650	0.55612	0.52633	H	-3.77803	2.86017	-1.29341
H	3.52993	3.33274	0.76806	H	-4.36455	1.23391	-0.70011
H	4.03111	1.59997	0.42770	H	-1.47305	2.20693	-1.20361
H	1.17915	2.69964	0.93902	H	-2.15191	-1.76280	-1.75456
H	2.74912	-1.66557	2.24994	H	-3.64962	-0.85779	-1.49269
H	4.00475	-0.54358	1.71924	H	-3.44995	-2.47122	-0.76821
H	4.01518	-2.22207	1.13719	H	-0.47614	-2.08817	0.14061
H	0.22242	-2.22439	0.21657	H	-1.80032	-2.82209	1.07276
H	1.54568	-3.20996	-0.44019	H	-0.85947	-1.48915	1.76165
H	0.65285	-2.10296	-1.49448	H	-4.20515	-0.00885	0.94646
H	4.24928	0.09516	-1.42588	H	-2.96218	-0.28154	2.22494
H	2.89336	-0.41233	-2.48859	H	-3.87653	-1.61560	1.54961
H	3.94872	-1.59111	-1.75013	C	2.07432	0.36655	0.20738
C	-0.88040	0.67876	-0.59866	C	2.38001	-0.42844	-0.89697
H	-0.52478	0.01492	-1.40529	C	3.10882	0.80858	1.03755
H	-0.84027	1.71106	-0.98778	C	3.70495	-0.77636	-1.16493
C	-2.30393	0.32049	-0.24539	H	1.57473	-0.76328	-1.54153
C	-3.30140	0.44815	-1.21699	C	4.42944	0.46056	0.77150
C	-2.64562	-0.14248	1.02475	H	2.87656	1.43142	1.89938
C	-4.62093	0.11570	-0.92705	C	4.73167	-0.33561	-0.33445
H	-3.04104	0.81221	-2.20919	H	3.93404	-1.39327	-2.02875
C	-3.96975	-0.47481	1.31616	H	5.22322	0.81102	1.42431
H	-1.86939	-0.23434	1.77651	H	5.76140	-0.60666	-0.54605
C	-4.95944	-0.34822	0.34489	C	-2.29870	-0.89424	0.22524
H	-5.38559	0.22090	-1.69074	C	0.65068	0.75349	0.53044
H	-4.22704	-0.83239	2.30877	H	0.56911	1.85181	0.59202
H	-5.98846	-0.60645	0.57525	H	0.37450	0.35232	1.51926
Li	2.47591	1.56738	-1.33331	Li	-2.79633	1.64882	1.15106

Electronic Energy = -878.793986136 Zero-point corrected electronic energy=-878.507387 Zero-point corrected Gibbs free energy=-878.555095	Electronic Energy = -627.388735965 Zero-point corrected electronic energy=-627.090779 Zero-point corrected Gibbs free energy=-627.135281
3aA-C^2Li	3aCA-C^2Li
C 2.29183 2.95979 -0.29554 C 2.00753 1.95513 0.53326 C 1.09112 0.81260 0.21844 Si 2.10009 -0.75546 -0.26916 C 2.66228 -1.66688 1.27085 C 1.11003 -1.94576 -1.40543 C 3.57899 -0.21881 -1.30674 O 0.27442 0.60314 1.36151 H 2.99791 3.73804 -0.02478 H 1.82337 3.03497 -1.27472 H 2.46978 1.91122 1.52022 H 1.80024 -1.96675 1.87272 H 3.28939 -1.01438 1.88687 H 3.24790 -2.55669 1.01769 H 0.68472 -2.79372 -0.84789 H 1.76906 -2.39465 -2.15588 H 0.33293 -1.42578 -1.98868 H 4.25960 0.41145 -0.72750 H 3.26104 0.36249 -2.17962 H 4.13586 -1.09162 -1.66444 C -0.64709 -0.46404 1.22655 H -0.69237 -1.04954 2.14907 C -1.92944 -0.11165 0.66569 C -2.18735 1.14274 0.04302 C -2.93342 -1.11370 0.49562 C -3.35907 1.36978 -0.66024 H -1.46042 1.93844 0.17525 C -4.11496 -0.86172 -0.20720 H -2.81639 -2.07034 1.01385 C -4.33752 0.37421 -0.80392 H -3.52572 2.34930 -1.10140 H -4.86634 -1.64395 -0.27894 H -5.24969 0.56849 -1.35688 H 0.47235 1.09676 -0.65582 Li -0.97583 -1.68082 -0.38300	C 1.34142 2.81168 -0.29828 C 1.46169 1.73807 0.47945 C 1.29397 0.31376 0.01155 C 3.36493 -0.50571 1.21472 C 2.43979 -1.84040 -0.67097 C 3.55062 0.32915 -1.14925 O 0.46117 -0.33024 0.94857 H 1.46296 3.81573 0.09564 H 1.10428 2.72013 -1.35653 H 1.66655 1.84960 1.54345 H 0.80562 0.33655 -0.98321 H 2.70545 -0.97012 1.95338 H 3.64256 0.48864 1.57763 H 4.28383 -1.09722 1.13522 H 1.79357 -2.41161 0.00652 H 3.39099 -2.37579 -0.75840 H 2.03136 -1.80977 -1.69959 H 3.81480 1.32458 -0.78502 H 3.04200 0.45203 -2.11424 H 4.47726 -0.22895 -1.32449 C -0.55085 -1.23178 0.43357 H -0.65209 -2.00849 1.20528 C -1.86208 -0.56879 0.24414 C -2.02194 0.82547 0.16514 C -3.01632 -1.35853 0.05321 C -3.26666 1.39354 -0.10972 H -1.16456 1.46734 0.34073 C -4.25505 -0.79059 -0.21213 H -2.92949 -2.44298 0.12903 C -4.39280 0.59797 -0.30526 H -3.35542 2.47590 -0.16153 H -5.12292 -1.43247 -0.34113 H -5.35921 1.04527 -0.51455 C 2.66458 -0.41508 -0.14525 Li 0.05511 -2.11634 -1.26745
Electronic Energy = -878.77102645 Zero-point corrected electronic energy=-878.485151 Zero-point corrected Gibbs free energy=-878.531583	Electronic Energy = -627.37229291 Zero-point corrected electronic energy=-627.075641 Zero-point corrected Gibbs free energy=-627.120203
Anionic Intermediates	

3aA-C^1_anion			
C	3.11448	2.65205	0.46936
C	1.87808	2.04738	0.54156
C	1.42961	0.74602	0.24515
Si	2.35305	-0.76391	-0.14491
C	2.84258	-1.84815	1.35611
C	1.30313	-1.93171	-1.22680
C	3.98652	-0.42791	-1.05635
O	0.03629	0.50072	0.54712
H	3.22972	3.69226	0.75323
H	4.00311	2.13065	0.12611
H	1.06694	2.69331	0.90407
H	1.94562	-2.17017	1.89793
H	3.46031	-1.26738	2.05050
H	3.40414	-2.74306	1.05523
H	0.30702	-2.05582	-0.78422
H	1.76467	-2.92401	-1.30850
H	1.17564	-1.52615	-2.23675
H	4.74379	-0.03261	-0.37070
H	3.84126	0.30650	-1.85521
H	4.37614	-1.35627	-1.49335
C	-0.81525	0.82256	-0.51303
H	-0.46774	0.33787	-1.44216
H	-0.80581	1.90917	-0.70765
C	-2.22832	0.37639	-0.21262
C	-3.26786	0.70102	-1.09118
C	-2.52203	-0.37645	0.92625
C	-4.57214	0.28176	-0.84371
H	-3.04636	1.28995	-1.97953
C	-3.82924	-0.79595	1.17768
H	-1.70828	-0.61675	1.60248
C	-4.85890	-0.47085	0.29668
H	-5.36665	0.54260	-1.53805
H	-4.04462	-1.37964	2.06889
H	-5.87578	-0.79834	0.49488
Electronic Energy = -871.265577139 Zero-point corrected electronic energy=-870.983479 Zero-point corrected Gibbs free energy=-871.030919			

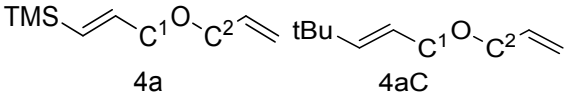
3aCA-C^1_anion			
C	3.64674	2.09399	0.67728
C	2.34400	1.62814	0.54856
C	1.71473	0.51420	-0.01839
C	2.38575	-1.64123	1.07520
C	1.46475	-1.66348	-1.24787
C	3.73574	-0.74700	-0.83225
O	0.33435	0.37336	0.38071
H	3.80926	3.07105	1.12107
H	4.51731	1.60647	0.25725
H	1.59709	2.30465	0.98119
H	1.37647	-1.75642	1.48716
H	2.99029	-1.08249	1.79888
H	2.82524	-2.64225	0.94403
H	0.42878	-1.73930	-0.89825
H	1.86306	-2.68200	-1.36323
H	1.46365	-1.17791	-2.23143
H	4.43811	-0.36978	-0.08557
H	3.74724	-0.06591	-1.69078
H	4.08522	-1.73727	-1.15799
C	-1.97904	0.43668	-0.20790
C	-2.20781	-0.56596	0.73756
C	-3.07699	1.00236	-0.86535
C	-3.50663	-0.99426	1.01460
H	-1.34961	-0.99025	1.24860
C	-4.37406	0.57505	-0.59266
H	-2.90858	1.78947	-1.59821
C	-4.59483	-0.42853	0.35228
H	-3.66860	-1.77293	1.75537
H	-5.21417	1.02812	-1.11268
H	-5.60561	-0.76176	0.57108
C	2.31929	-0.85540	-0.25519
C	-0.57440	0.88703	-0.54350
H	-0.53815	1.99022	-0.56336
H	-0.31534	0.55192	-1.56294
Electronic Energy = -619.856504589 Zero-point corrected electronic energy=-619.563499 Zero-point corrected Gibbs free energy=-619.60761			

3aA-C^2_anion			
C	4.11713	1.61444	0.26317
C	2.81902	1.48597	0.56880
C	1.72976	1.05462	-0.34377
Si	1.27334	-0.87000	-0.18860
C	1.34772	-1.90952	1.42296
C	0.02928	-1.50557	-1.48777
C	2.93692	-1.54425	-0.98662

3aCA-C^2_anion			
C	1.48081	2.67713	-0.73164
C	1.39227	1.69100	0.16143
C	1.36764	0.22163	-0.16616
C	3.31752	-0.24445	1.38091
C	2.57774	-1.96059	-0.27577
C	3.73108	0.11036	-1.06780
O	0.44990	-0.40801	0.71405

O	0.47001	1.60663	0.03185	H	1.47151	3.72150	-0.43291
H	4.86003	1.85416	1.01817	H	1.53669	2.46645	-1.79771
H	4.47338	1.45700	-0.75300	H	1.29924	1.92100	1.22332
H	2.49829	1.65275	1.60003	H	1.01917	0.08501	-1.20222
H	0.33903	-2.07345	1.81870	H	2.58139	-0.56496	2.12507
H	1.91283	-1.35347	2.18309	H	3.55753	0.81025	1.55875
H	1.84490	-2.87618	1.27828	H	4.23698	-0.82725	1.52074
H	-0.88713	-1.86681	-1.00804	H	1.91355	-2.39219	0.47799
H	0.45357	-2.30125	-2.11059	H	3.54787	-2.47220	-0.23092
H	-0.27069	-0.67738	-2.14219	H	2.13183	-2.14430	-1.26047
H	3.81501	-1.31283	-0.36873	H	3.89162	1.18305	-0.91974
H	3.11331	-1.10900	-1.98143	H	3.34773	-0.03964	-2.08485
H	2.89399	-2.63594	-1.10853	H	4.70179	-0.39594	-0.99402
C	-0.19666	0.53791	0.70860	C	-0.59592	-1.13894	0.11760
H	-0.01383	0.58772	1.79622	H	-0.37714	-2.18445	-0.08667
C	-1.61896	0.45171	0.41277	C	-1.87176	-0.60717	0.07635
C	-2.19630	1.06700	-0.71921	C	-2.18657	0.73821	0.49530
C	-2.47117	-0.34863	1.20871	C	-3.00394	-1.36746	-0.40398
C	-3.53470	0.86944	-1.04442	C	-3.47112	1.24656	0.41004
H	-1.56266	1.69969	-1.33339	H	-1.38281	1.35764	0.88293
C	-3.80456	-0.54728	0.87585	C	-4.27290	-0.83033	-0.47528
H	-2.05916	-0.82438	2.09737	H	-2.83652	-2.39554	-0.72306
C	-4.35657	0.05739	-0.25894	C	-4.55081	0.49196	-0.07703
H	-3.94580	1.35721	-1.92630	H	-3.64380	2.27235	0.73818
H	-4.42579	-1.17716	1.50957	H	-5.08270	-1.45732	-0.85017
H	-5.39991	-0.09725	-0.51852	H	-5.55283	0.90460	-0.13832
H	1.96833	1.32424	-1.38590	C	2.75926	-0.45858	-0.03036
Electronic Energy = -871.263020881 Zero-point corrected electronic energy=-870.981334 Zero-point corrected Gibbs free energy=-871.026268				Electronic Energy = -619.863870041 Zero-point corrected electronic energy=-619.571761 Zero-point corrected Gibbs free energy=-619.616343			

Numbering system followed for structures 4a and 4aC to 6b and 6bC



Silicon Analogues				**Carbon Analogues**			
4a_Reactant				4aC_Reactant			
C	-5.50307800	0.19763600	0.07495800	C	5.26147200	-0.11168000	0.20617300
C	-4.31257000	0.24536300	-0.51738400	C	4.12371700	0.07835400	-0.45705600
C	-3.02701800	0.47850700	0.21418200	C	2.81631000	-0.53506700	-0.06126600
O	-2.10176900	-0.51938400	-0.16364000	O	1.82976600	0.47379400	-0.03316500
C	-0.84111600	-0.34572900	0.44578300	C	0.54993200	-0.03385400	0.28009800
C	0.05085700	-1.47602200	0.02171900	C	-0.40820100	1.12385600	0.29556100
C	1.37088300	-1.39046400	-0.18418100	C	-1.73765700	1.10260000	0.17074000

Si	2.46420000	0.13839300	-0.04208800	C	-2.58339600	-0.55145600	-1.50279200
C	2.08915000	1.35559700	-1.43212400	C	-2.33370300	-1.25521000	0.90131200
C	2.23383900	0.98622500	1.62742600	C	-4.10172100	0.37195600	0.25368300
C	4.24809000	-0.44297500	-0.19458500	H	6.19544100	0.32556100	-0.13123300
H	-6.41573000	0.05396300	-0.49396600	H	5.29445100	-0.71471100	1.11041800
H	-5.60306600	0.30208500	1.15277300	H	4.09970100	0.69501400	-1.35384400
H	-4.22281700	0.12567800	-1.59573100	H	2.90228800	-1.02161800	0.92360700
H	-3.19441500	0.45849600	1.30307900	H	2.52701500	-1.30926700	-0.79320900
H	-2.62006600	1.47141500	-0.04469800	H	0.58048900	-0.53012300	1.26602100
H	-0.95735300	-0.34970500	1.54456000	H	0.25876800	-0.79457300	-0.46136400
H	-0.41367000	0.63009500	0.16389200	H	0.08712300	2.08355300	0.43105800
H	-0.47497600	-2.42548500	-0.08826600	H	-2.23719600	2.07128200	0.20351400
H	1.87112300	-2.32259900	-0.45539300	H	-1.57311200	-0.88404600	-1.76010400
H	1.05511600	1.71222600	-1.39797400	H	-2.85161600	0.26279300	-2.18338400
H	2.24597100	0.88521400	-2.40769000	H	-3.27304600	-1.38581700	-1.67587400
H	2.74856200	2.22768800	-1.36572100	H	-1.36915300	-1.71457200	0.67011500
H	1.23265600	1.41333200	1.74095500	H	-3.09736400	-2.03541200	0.80681700
H	2.95726100	1.80075300	1.74210900	H	-2.31249800	-0.92182300	1.94410100
H	2.39177100	0.27766000	2.44677000	H	-4.38770300	1.20359300	-0.39947300
H	4.41515800	-0.94769100	-1.15183700	H	-4.20089000	0.70619800	1.29230900
H	4.50291500	-1.14552600	0.60559600	H	-4.80926800	-0.44748900	0.08955400
H	4.94269300	0.40114300	-0.13487400	C	-2.66534400	-0.08598200	-0.03873800
Electronic Energy = -718.263923904 Zero-point corrected electronic energy=-718.014271 Zero-point corrected Gibbs free energy=-718.058966				Electronic Energy = -466.866997393 Zero-point corrected electronic energy=-466.605546 Zero-point corrected Gibbs free energy=-466.645999			

Lithiated Intermediates

4aA-C[1]Li				4aCA-C[1]Li			
C	-5.51393200	-0.15577800	-0.42671900	C	-5.51393200	-0.15577800	-0.42671900
C	-4.45958700	-0.23041300	0.38166900	C	-4.45958700	-0.23041300	0.38166900
C	-3.05807000	-0.46850700	-0.09025500	C	-3.05807000	-0.46850700	-0.09025500
O	-2.20599000	0.48546700	0.50611900	O	-2.20599000	0.48546700	0.50611900
C	-0.86018700	0.27080100	0.22882600	C	-0.86018700	0.27080100	0.22882600
C	-0.05292300	1.35556800	-0.05282900	C	-0.05292300	1.35556800	-0.05282900
C	1.33469600	1.33526600	-0.35398400	C	1.33469600	1.33526600	-0.35398400
Si	2.48039100	-0.04732000	0.03868000	Si	2.48039100	-0.04732000	0.03868000
C	2.48744400	-0.60469200	1.84183700	C	2.48744400	-0.60469200	1.84183700
C	1.97358200	-1.61110700	-0.97843900	C	1.97358200	-1.61110700	-0.97843900
C	4.22557400	0.38553200	-0.51510100	C	4.22557400	0.38553200	-0.51510100
H	-6.51736400	-0.01241000	-0.03954800	H	-6.51736400	-0.01241000	-0.03954800
H	-5.40601100	-0.23629400	-1.50589300	H	-5.40601100	-0.23629400	-1.50589300
H	-4.57910100	-0.13264300	1.45947100	H	-4.57910100	-0.13264300	1.45947100
H	-2.99854400	-0.40246400	-1.18943300	H	-2.99854400	-0.40246400	-1.18943300
H	-2.73420600	-1.48278300	0.20111600	H	-2.73420600	-1.48278300	0.20111600
H	-0.46190200	-0.66753600	0.63020600	H	-0.46190200	-0.66753600	0.63020600

H	-0.60093400	2.28994900	-0.19476700
H	1.77987300	2.29683000	-0.59560900
H	1.47055100	-0.78314200	2.20619100
H	2.92629100	0.17698700	2.46981700
H	3.06734100	-1.52360300	1.98098400
H	0.98858800	-2.03332300	-0.73445900
H	2.68898300	-2.41057600	-0.75881200
H	2.04091700	-1.45620600	-2.06743300
H	4.59290400	1.26161900	0.02895500
H	4.24928600	0.62148100	-1.58386500
H	4.91888800	-0.44142100	-0.33087100
Li	0.34576900	0.01807900	-1.59218400

Electronic Energy = -725.1909235
Zero-point corrected electronic energy=-724.952723
Zero-point corrected Gibbs free energy=-724.997035

C	4.22557400	0.38553200	-0.51510100
H	-6.51736400	-0.01241000	-0.03954800
H	-5.40601100	-0.23629400	-1.50589300
H	-4.57910100	-0.13264300	1.45947100
H	-2.99854400	-0.40246400	-1.18943300
H	-2.73420600	-1.48278300	0.20111600
H	-0.46190200	-0.66753600	0.63020600
H	-0.60093400	2.28994900	-0.19476700
H	1.77987300	2.29683000	-0.59560900
H	1.47055100	-0.78314200	2.20619100
H	2.92629100	0.17698700	2.46981700
H	3.06734100	-1.52360300	1.98098400
H	0.98858800	-2.03332300	-0.73445900
H	2.68898300	-2.41057600	-0.75881200
H	2.04091700	-1.45620600	-2.06743300
H	4.59290400	1.26161900	0.02895500
H	4.24928600	0.62148100	-1.58386500
H	4.91888800	-0.44142100	-0.33087100
Li	0.34576900	0.01807900	-1.59218400

Electronic Energy = -473.7816216
Zero-point corrected electronic energy=-473.531787
Zero-point corrected Gibbs free energy=-473.573145

4aA-C^2Li

C	-4.07440400	-1.57804800	0.10035500
C	-3.07125500	-0.66217900	0.32668300
C	-2.94022600	0.68161600	-0.08588200
O	-1.59385400	1.07506200	-0.45451000

4aCA-C^2Li

C	5.18291800	0.44350000	-0.01780800
C	3.99096600	-0.29219900	-0.13695800
C	2.76022300	0.04351000	0.41138100
O	1.68604000	-0.82276200	0.22226100

C	0.48308800	2.13124500	0.01554100	C	-0.58660400	-1.21630500	-0.23845200
C	1.61833200	1.47095900	-0.25058000	C	-1.91522100	-1.08011400	-0.22313100
Si	1.97332600	-0.36175400	0.00642400	C	-2.82929100	0.47445400	1.50102100
C	2.12304800	-0.82414400	1.82341700	C	-2.20166700	1.39004300	-0.75536600
C	0.59561500	-1.40071200	-0.78703200	C	-4.17287500	-0.11022500	-0.52507800
C	3.58754700	-0.74200900	-0.88007100	H	6.07685100	0.08971600	-0.51395000
H	-4.09239500	-2.51835000	0.63822000	H	5.34997800	1.04318100	0.87933700
H	-4.96717200	-1.30239700	-0.45506600	H	3.95037100	-1.08777200	-0.88419500
H	-3.68458000	1.22352700	-0.65965100	H	2.70634600	0.64076900	1.33170800
H	0.39233400	3.18542700	-0.24804600	H	-0.16908200	-2.20972400	-0.39286300
H	2.41806300	2.05201900	-0.71655600	H	-2.49209300	-1.99597500	-0.35693800
H	1.19654200	-0.63305600	2.37305900	H	-1.83483800	0.66925900	1.91468400
H	2.92039900	-0.24708000	2.30164700	H	-3.25921200	-0.37155400	2.04679400
H	2.36549000	-1.88700300	1.92868100	H	-3.45694200	1.35503400	1.68258100
H	-0.29919100	-1.38402800	-0.15418900	H	-1.25116700	1.73480100	-0.34039300
H	0.38006700	-1.00829600	-1.78987100	H	-2.91085700	2.22243000	-0.68277500
H	0.89682300	-2.44713800	-0.89640600	H	-2.05076000	1.16050100	-1.81555700
H	3.84868000	-1.80073000	-0.78347700	H	-4.61492600	-0.97147200	-0.01242700
H	4.41035400	-0.15518900	-0.45865600	H	-4.15918800	-0.32485000	-1.59925500
H	3.52061900	-0.50619900	-1.94712300	H	-4.82340000	0.75474800	-0.35686700
C	-0.74972800	1.50806700	0.61212700	C	-2.75513000	0.16959300	-0.00526100
H	-1.31281300	2.22090800	1.22299900	Li	3.65093800	1.64787500	-0.70512000
H	-0.48906100	0.64850000	1.24797300	C	0.47352700	-0.16292500	-0.06525800
Li	-1.86354100	-0.48263400	-1.40681900	H	0.22226300	0.53401000	0.75065400
H	-2.22137200	-1.03772100	0.91571900	H	0.59443700	0.43938200	-0.98380300
Electronic Energy = -725.1777087 Zero-point corrected electronic energy=-724.940354 Zero-point corrected Gibbs free energy=-724.986922				Electronic Energy = -473.7796463 Zero-point corrected electronic energy=-473.530899 Zero-point corrected Gibbs free energy=-473.573601			
Anionic Intermediates							
4aA-C[1]_anion				4aCA-C[1]_anion			
C	5.47803800	0.26174600	0.55839200	C	-5.12625400	0.65918300	-0.09030000
C	4.47709100	-0.36231600	-0.06126300	C	-4.16606700	-0.26542700	-0.09279900
C	3.03208400	-0.26435600	0.33312800	C	-2.73022000	-0.01495100	-0.45617900
O	2.25316100	-0.06296100	-0.82120900	O	-1.90122300	-0.65360100	0.48170400
C	0.86565000	-0.09126200	-0.55741800	C	-0.52007000	-0.55245600	0.16556600
C	0.16472600	1.07321300	-0.41880700	C	0.22753100	0.44698900	0.76298800
C	-1.21470300	1.31001600	-0.17182100	C	1.57704600	0.80753400	0.73208100
Si	-2.46151600	0.03666600	0.09006600	C	2.79585200	-1.37417300	0.38933100
C	-2.72823100	-1.16926400	-1.37289000	C	2.33147500	0.11903300	-1.57379500
C	-2.13030200	-1.12618100	1.57485100	C	3.99431800	0.79238900	0.14940000
C	-4.16893300	0.82001300	0.41763900	H	-6.15670100	0.41584900	0.15420500
H	6.51161400	0.13412900	0.24923000	H	-4.90569700	1.69739000	-0.32924800
H	5.29005400	0.92840300	1.39716600	H	-4.39936500	-1.29661300	0.17385200
H	4.67974300	-1.00816400	-0.91575600	H	-2.52180800	1.06642500	-0.49762300
H	2.87892800	0.55065400	1.05841000	H	-2.53304600	-0.41979500	-1.46560400
H	2.72506600	-1.20206600	0.83047500	H	-0.16253000	-1.35463800	-0.47350900
H	0.44724000	-1.09622700	-0.50578700	H	-0.39301600	1.08308100	1.40445200

H	0.80319200	1.95842800	-0.53193000
H	-1.52505400	2.35314600	-0.13680800
H	-1.77174400	-1.59941600	-1.69137200
H	-3.14433800	-0.62882500	-2.23109400
H	-3.40785500	-1.99206600	-1.11442200
H	-1.12235300	-1.55157800	1.50376100
H	-2.85037000	-1.95338000	1.62540600
H	-2.18103600	-0.55993800	2.51199600
H	-4.47488000	1.44189000	-0.43156700
H	-4.14010100	1.45608200	1.30964600
H	-4.93468100	0.04962600	0.57054000

Electronic Energy = -717.6605292
Zero-point corrected electronic energy=-717.427673
Zero-point corrected Gibbs free energy=-717.473326

H	1.88878400	1.65913400	1.33181500
H	1.82710200	-1.88355700	0.35934900
H	3.15088400	-1.40503900	1.42569000
H	3.50528800	-1.93012600	-0.24387700
H	1.32663800	-0.27417200	-1.76150800
H	3.05562800	-0.47377600	-2.15440300
H	2.35219400	1.15304200	-1.93670600
H	4.26064400	0.78617500	1.21399700
H	3.93642600	1.83786100	-0.17892300
H	4.79666100	0.29396900	-0.41254500
C	2.64667200	0.09414600	-0.06346800

Electronic Energy = -466.2470748
Zero-point corrected electronic energy=-466.003054
Zero-point corrected Gibbs free energy=-466.044017

4aA-C^2_anion

C	5.45707400	-0.68322800	0.30823300
C	4.22867600	-0.03199900	0.24859700
C	3.10344200	-0.24118400	-0.53469300
O	2.08572300	0.75677500	-0.53376000
C	-0.05604100	1.50412700	0.12907900
C	-1.39522000	1.41193600	0.11530300
Si	-2.39108700	-0.17172000	0.03053100
C	-2.24839000	-0.99954900	-1.66024900
C	-1.89767500	-1.39809500	1.37558900
C	-4.20646300	0.29391100	0.30017700
H	6.19323000	-0.40310500	1.05347700
H	5.69153400	-1.52782300	-0.33522400
H	4.09921700	0.79927700	0.95296000
H	3.08325000	-0.87560500	-1.41926900
H	0.43211900	2.48007900	0.17278500
H	-1.95430100	2.34991500	0.16356300
H	-1.20912600	-1.24880700	-1.89381600
H	-2.61700000	-0.33138600	-2.44539800
H	-2.83749300	-1.92323300	-1.69028300
H	-0.86089200	-1.72747700	1.25787500
H	-2.54273700	-2.28387300	1.34680400
H	-1.99120900	-0.93950700	2.36568800
H	-4.54712600	1.00388200	-0.46156400
H	-4.34755900	0.76037900	1.28131100
H	-4.85183900	-0.58996700	0.25062500
C	0.91770500	0.35707700	0.12419700
H	0.47909000	-0.53385900	-0.35880200
H	1.15163400	0.06301100	1.16451200

Electronic Energy = -717.6390499
Zero-point corrected electronic energy=-717.406322

4aCA-C^2_anion

C	-5.19268700	-0.67612900	-0.27116800
C	-3.93601100	-0.07387600	-0.30784200
C	-2.91405600	0.00397500	0.62230800
O	-1.81046700	0.86155500	0.35913700
C	0.42346400	1.18790400	-0.31560900
C	1.75367600	1.04994700	-0.34240100
C	2.62372800	-0.41573900	1.49152200
C	2.04472300	-1.44169800	-0.72919300
C	4.02007600	0.05809900	-0.52330200
H	-5.83604200	-0.66155500	-1.14377600
H	-5.54465000	-1.21801400	0.60338500
H	-3.68516500	0.43910200	-1.24493900
H	-2.99409400	-0.30079600	1.66406000
H	0.00568900	2.16641600	-0.55221400
H	2.33563700	1.93828600	-0.59577600
H	1.61680700	-0.57381500	1.88768900
H	3.05299200	0.45406400	2.00070200
H	3.23412600	-1.29500800	1.73487000
H	1.06093500	-1.72898400	-0.35182000
H	2.72725800	-2.28548800	-0.56605200
H	1.95518900	-1.27334100	-1.80770300
H	4.45219800	0.94557300	-0.04608400
H	4.03573000	0.21491000	-1.60807100
H	4.66167700	-0.80016400	-0.29157400
C	2.58690600	-0.18652100	-0.02941000
C	-0.64527700	0.17070900	-0.00624100
H	-0.33613500	-0.51292100	0.80254700
H	-0.84567000	-0.46073600	-0.89032200

Electronic Energy = -466.2405119
Zero-point corrected electronic energy=-465.996509

Zero-point corrected Gibbs free energy=-717.451354				Zero-point corrected Gibbs free energy=-466.03768			
4b_Reactant				4bC_Reactant			
C	-5.26155	-0.78470	-0.09995	C	5.05130	-0.70607	0.02512
C	-3.96175	-1.01246	0.07077	C	3.74937	-0.98065	0.01880
C	-2.88211	-0.13114	-0.47919	C	2.69419	-0.02671	0.49034
O	-1.97925	0.17276	0.56475	O	1.68933	0.05107	-0.49989
C	-0.74676	0.73445	0.13735	C	0.47866	0.65969	-0.06601
C	0.15313	0.74234	1.34228	C	-0.50430	0.45146	-1.18539
C	1.43959	0.37326	1.35629	C	-1.77865	0.05573	-1.12426
Si	2.45669	-0.31801	-0.07290	C	-2.09992	-1.67579	0.66603
C	1.83317	-2.02916	-0.56042	C	-2.62553	0.73822	1.17070
C	2.41315	0.82024	-1.57832	C	-4.06291	-0.55629	-0.39061
C	4.23409	-0.45410	0.53314	H	5.78741	-1.43399	-0.29997
H	-6.01299	-1.46315	0.29025	H	5.42321	0.26014	0.35769
H	-5.61576	0.09166	-0.63771	H	3.38528	-1.94492	-0.33138
H	-3.61786	-1.88400	0.62516	H	3.14181	0.95743	0.69046
H	-3.32381	0.77928	-0.90914	H	2.25012	-0.39385	1.43233
H	-2.34224	-0.65839	-1.28522	C	0.66814	2.15193	0.21785
C	-0.92575	2.15005	-0.41563	H	0.14644	0.15230	0.85128
H	-0.31849	0.08906	-0.64768	H	-0.08081	0.67829	-2.16389
H	-0.33609	1.11530	2.24461	H	-2.30088	-0.00925	-2.07967
H	1.95572	0.47752	2.31329	H	-1.06770	-1.59038	1.01737
H	0.78896	-2.00445	-0.88782	H	-2.12953	-2.46555	-0.09119
H	1.89849	-2.71860	0.28694	H	-2.72440	-1.98628	1.51191
H	2.43475	-2.43860	-1.37922	H	-1.64173	0.87914	1.62559
H	1.42363	0.85300	-2.04562	H	-3.32255	0.46081	1.96987
H	3.12532	0.46808	-2.33285	H	-2.94810	1.69857	0.75481
H	2.69148	1.84301	-1.30430	H	-4.11406	-1.32935	-1.16501
H	4.30153	-1.11242	1.40555	H	-4.47370	0.37022	-0.80677
H	4.62823	0.52628	0.82040	H	-4.70097	-0.86755	0.44310
H	4.88500	-0.86265	-0.24652	H	1.05736	2.64766	-0.67704
H	-1.39422	2.78526	0.34277	H	1.36515	2.32191	1.04378
H	-1.55075	2.15678	-1.31361	H	-0.28961	2.60924	0.47990
H	0.04816	2.57438	-0.67474	C	-2.61658	-0.34870	0.08343
Electronic Energy = -757.564439 Zero-point corrected electronic energy=-757.286926 Zero-point corrected Gibbs free energy=-757.333369				Electronic Energy = -506.1664721 Zero-point corrected electronic energy=-505.877115 Zero-point corrected Gibbs free energy=-505.919195			
Lithiated Intermediates							
4bA-C^{1}Li				4bCA-C^{1}Li			
C	5.63436	0.29855	0.24506	C	5.33029	0.13262	0.20603
C	4.54155	-0.45618	0.16129	C	4.21894	-0.54179	-0.07887
C	3.15627	0.04242	0.43924	C	2.86574	-0.20179	0.46931

O	2.30776	-0.36720	-0.61080	O	1.93683	-0.18437	-0.58801
C	0.94964	-0.08023	-0.40711	C	0.61193	0.14430	-0.19087
C	0.08147	-1.11146	-0.71413	C	-0.31501	-0.82749	-0.62770
C	-1.32656	-1.22097	-0.53335	C	-1.67389	-1.05789	-0.39691
Si	-2.62041	-0.03692	0.01184	C	-4.08377	-0.86488	0.13697
C	-2.08400	0.76016	1.69332	C	-2.49880	0.50678	1.44450
C	-3.14986	1.39581	-1.10601	C	-2.96300	1.04931	-0.98566
C	-4.17942	-1.02683	0.39356	H	6.29544	-0.16763	-0.18899
H	6.62311	-0.11102	0.06588	H	5.30906	1.01233	0.84503
H	5.57403	1.35487	0.49649	H	4.25108	-1.41017	-0.73515
H	4.61346	-1.50858	-0.10865	H	2.90343	0.76798	0.99094
H	3.16595	1.13791	0.54668	H	2.55988	-0.96307	1.21127
H	2.78452	-0.38364	1.39018	C	0.44019	1.65029	-0.21788
C	0.62963	1.39332	-0.45035	H	0.20550	-1.70085	-1.02851
H	0.60743	-2.03010	-0.98533	H	-2.04694	-1.99487	-0.80185
H	-1.73653	-2.17274	-0.86711	H	-3.99789	-1.68875	0.85467
H	-2.05722	0.03007	2.51917	H	-4.34441	-1.29223	-0.83676
H	-2.84997	1.48629	1.98474	H	-4.90505	-0.21251	0.45426
H	-1.14209	1.32631	1.68120	H	-2.56389	-0.28388	2.20988
H	-2.35848	2.12555	-1.29648	H	-3.25234	1.25391	1.71450
H	-3.99876	1.92786	-0.66040	H	-1.53230	1.02325	1.52981
H	-3.47228	0.99954	-2.07452	H	-3.26030	0.61763	-1.94620
H	-3.98093	-1.81615	1.12539	H	-2.04539	1.61565	-1.15325
H	-4.55897	-1.50365	-0.51636	H	-3.74904	1.74392	-0.66197
H	-4.97193	-0.38229	0.78775	H	0.54387	2.02957	-1.24531
H	1.20303	1.84741	-1.27004	H	1.21927	2.13333	0.38182
H	0.87993	1.94964	0.46261	H	-0.51903	1.99929	0.16493
H	-0.42882	1.55420	-0.66165	C	-2.76597	-0.08346	0.03993
Li	-0.39676	-0.78153	1.25731	Li	-0.52180	-0.81462	1.38394
Electronic Energy = -764.4853254 Zero-point corrected electronic energy=-764.218671 Zero-point corrected Gibbs free energy=-764.264271				Electronic Energy = -513.0716536 Zero-point corrected electronic energy=-512.793592 Zero-point corrected Gibbs free energy=-512.835755			
4bA-C^2Li				4bCA-C^2Li			
C	-2.62443	-2.61650	0.17113	C	4.45017	-1.41849	0.16378
C	-2.80342	-1.21937	0.21871	C	3.30412	-0.87252	-0.43285
C	-2.34860	-0.29656	-0.70010	C	2.68430	0.32403	-0.08081
O	-2.32279	1.07426	-0.38859	O	1.56675	0.72769	-0.81009
C	-0.49278	0.79569	1.13977	C	-0.74064	1.06278	-1.01968
C	0.64698	0.09081	1.26992	C	-1.93449	0.46486	-0.97266
Si	1.97139	-0.26619	-0.03196	C	-1.70970	-1.83306	0.02132
C	1.27753	-1.52725	-1.27184	C	-2.46157	0.08480	1.48054
C	2.54588	1.27348	-0.94313	C	-3.95493	-0.80076	-0.29881
C	3.41980	-1.05293	0.86891	H	4.82822	-2.37317	-0.17682
H	-3.08573	-3.23528	0.93002	H	5.18995	-0.74911	0.60863
H	-2.47573	-3.09609	-0.79922	H	2.71107	-1.51217	-1.09027
H	-3.12730	-0.79359	1.17195	H	3.28212	1.14019	0.34372
H	-2.19837	-0.52884	-1.75607	C	0.52977	2.28221	0.75064

C	-1.04498	3.01267	0.12523	H	-0.52295	1.71280	-1.86739
H	-1.15938	0.90890	1.99975	H	-2.61098	0.68182	-1.80031
H	0.84692	-0.30695	2.26856	H	-0.64962	-1.68739	0.24844
H	1.04183	-2.49507	-0.80509	H	-1.77438	-2.28545	-0.97325
H	2.03265	-1.74836	-2.03319	H	-2.12562	-2.54071	0.74832
H	0.39664	-1.15414	-1.81097	H	-1.44258	0.25150	1.83972
H	1.77016	1.69658	-1.58710	H	-2.95563	-0.59816	2.18172
H	3.41098	1.03398	-1.57079	H	-2.98954	1.04379	1.50836
H	2.85149	2.04612	-0.23049	H	-4.03069	-1.23090	-1.30333
H	3.10851	-1.95056	1.41317	H	-4.55422	0.11595	-0.27492
H	3.85467	-0.35582	1.59230	H	-4.39195	-1.51278	0.40928
H	4.20753	-1.34241	0.16621	H	0.68969	3.11648	0.06053
H	-1.67379	3.24972	0.98848	H	1.37961	2.23311	1.43909
H	-1.47231	3.49787	-0.75555	H	-0.37839	2.47608	1.32884
H	-0.03886	3.40394	0.30076	C	-2.49071	-0.50758	0.06182
Li	-0.79212	-1.59372	0.10815	Li	3.03591	-0.94917	1.59725
C	-1.00564	1.50790	-0.09498	C	0.39730	0.98059	-0.03992
H	-0.35282	1.27597	-0.95271	H	0.26253	0.14286	0.65841
Electronic Energy =				Electronic Energy = -513.0716536			
Zero-point corrected electronic energy=-764.226396				Zero-point corrected electronic energy=-512.802782			
Zero-point corrected Gibbs free energy=-764.270105				Zero-point corrected Gibbs free energy=-512.846127			
Anionic Intermediates							
4bA-C[1]_anion				4bCA-C[1]_anion			
C	5.08134	-1.72300	0.23116	C	5.30460	-0.00693	0.39164
C	4.51606	-0.58441	-0.16835	C	4.18005	-0.52968	-0.09678
C	3.24743	-0.01651	0.39642	C	2.79937	-0.24761	0.42381
O	2.41830	0.40022	-0.66332	O	1.93326	-0.05801	-0.66107
C	1.23435	1.03489	-0.21401	C	0.58219	0.21591	-0.25305
C	0.06677	0.33185	-0.18714	C	-0.30252	-0.83207	-0.48574
C	-1.22338	0.74006	0.25618	C	-1.67852	-1.07102	-0.41966
Si	-2.71996	-0.23603	0.04091	C	-2.43362	0.32462	1.53385
C	-2.33774	-2.07137	-0.30826	C	-3.00049	1.06477	-0.82257
C	-3.86504	-0.18828	1.57153	C	-4.08555	-0.92706	0.16189
C	-3.90345	0.26572	-1.38700	H	6.28074	-0.27470	-0.00326
H	6.01527	-2.07954	-0.19395	H	5.28121	0.71312	1.20718
H	4.61850	-2.34003	0.99810	H	4.21959	-1.23268	-0.92912
H	4.97850	0.01098	-0.95571	H	2.81812	0.63392	1.08818
H	3.49563	0.84488	1.04258	H	2.45240	-1.10119	1.03217
H	2.73304	-0.76053	1.02504	C	0.35568	1.69735	-0.21798
C	1.38929	2.46426	0.19710	H	0.25721	-1.72307	-0.79011
H	0.16502	-0.69095	-0.56801	H	-1.99042	-2.09368	-0.62244
H	-1.30762	1.73562	0.69827	H	-1.39907	0.67224	1.60324
H	-1.79248	-2.18803	-1.25185	H	-2.53033	-0.51885	2.22802
H	-3.26733	-2.64923	-0.38362	H	-3.10596	1.13024	1.86789
H	-1.72416	-2.50353	0.48976	H	-2.07820	1.61818	-1.00526
H	-3.37211	-0.65689	2.43020	H	-3.74552	1.75694	-0.39779
H	-4.82040	-0.69818	1.39107	H	-3.36567	0.71179	-1.79345

H	-4.08362	0.85170	1.84427
H	-3.37701	0.20643	-2.34664
H	-4.23347	1.30396	-1.25921
H	-4.79646	-0.37309	-1.43836
H	2.24287	2.92012	-0.32250
H	0.48554	3.02806	-0.07273
H	1.53946	2.62167	1.28132

Electronic Energy = -756.9624472
Zero-point corrected electronic energy=-756.701521
Zero-point corrected Gibbs free energy=-756.749619

H	-3.99281	-1.79432	0.82676
H	-4.35721	-1.29175	-0.83666
H	-4.90195	-0.29140	0.53231
H	1.20199	2.20278	0.27019
H	-0.54149	1.98235	0.33691
H	0.26759	2.15048	-1.22863
C	-2.76056	-0.15266	0.10167

Electronic Energy = -505.5404472
Zero-point corrected electronic energy=-505.268179
Zero-point corrected Gibbs free energy=-505.311787

4bA-C^2_anion

C	4.21620	-1.97971	0.25836
C	3.23160	-1.11162	-0.19989
C	2.96160	0.22082	0.08481
O	2.00235	0.89243	-0.72339
C	-0.26051	1.41389	-1.11194
C	-1.47586	0.84581	-1.15308
Si	-2.12411	-0.44443	0.04575
C	-1.11673	-2.03368	-0.02606
C	-2.18337	0.18999	1.82503
C	-3.90339	-0.83201	-0.47943
H	4.22672	-3.01720	-0.05650
H	4.97229	-1.66436	0.97343
H	2.51663	-1.53772	-0.91478
H	3.65026	0.88340	0.60538
C	0.93091	2.39237	0.85422
H	0.05244	2.11613	-1.88942
H	-2.12843	1.13097	-1.98255
H	-0.06738	-1.86005	0.23533
H	-1.13900	-2.45392	-1.03701
H	-1.52366	-2.78090	0.66512
H	-1.17671	0.35575	2.22097
H	-2.68641	-0.53699	2.47325
H	-2.73040	1.13721	1.88199
H	-3.93369	-1.21054	-1.50710
H	-4.53143	0.06469	-0.43244
H	-4.34868	-1.59170	0.17243
H	1.20788	3.27119	0.26048
H	1.72632	2.18787	1.57851
H	-0.00171	2.60422	1.38963
C	0.78561	1.17421	-0.06011
H	0.51732	0.30410	0.55843

Electronic Energy = -756.9417282
Zero-point corrected electronic energy=-756.680867
Zero-point corrected Gibbs free energy=-

4bCA-C^2_anion

C	4.30856	-1.71467	0.32714
C	3.20485	-1.00852	-0.14394
C	2.84307	0.32602	-0.04420
O	1.72464	0.78298	-0.79319
C	-0.59283	1.07159	-0.99485
C	-1.79234	0.47988	-0.96517
C	-1.58234	-1.82830	0.00496
C	-2.30804	0.07500	1.48759
C	-3.82295	-0.77179	-0.29256
H	4.38899	-2.78370	0.16545
H	5.10208	-1.23092	0.89174
H	2.46377	-1.60080	-0.69588
H	3.49984	1.11625	0.31249
C	0.66095	2.27084	0.79944
H	-0.36566	1.71444	-1.84703
H	-2.46177	0.69127	-1.80170
H	-0.52067	-1.68979	0.22460
H	-1.65892	-2.26975	-0.99445
H	-1.99731	-2.54052	0.72976
H	-1.28274	0.22221	1.83406
H	-2.80379	-0.61259	2.18485
H	-2.82357	1.04116	1.53006
H	-3.90862	-1.18863	-1.30275
H	-4.41259	0.15193	-0.25422
H	-4.26312	-1.48897	0.40995
H	0.77223	3.12830	0.12551
H	1.54903	2.20083	1.43586
H	-0.22492	2.42664	1.42544
C	-2.35351	-0.49780	0.06178
C	0.55248	0.98362	-0.02219
H	0.44330	0.13352	0.66378

Electronic Energy = -505.5419897
Zero-point corrected electronic energy=-505.269952
Zero-point corrected Gibbs free energy=-

756.726807				505.312845			
5a_Reactant				5aC_Reactant			
C	-5.05973	-0.17140	-0.41220	C	4.83478	-0.31107	0.08947
C	-3.79406	-0.47274	-0.71041	C	3.60409	-0.72116	0.40419
C	-2.56361	0.21160	-0.19761	C	2.35229	0.10279	0.40396
O	-1.58022	-0.77387	0.04881	O	1.30699	-0.68556	-0.12716
C	-0.36598	-0.22013	0.50337	C	0.06725	-0.01160	-0.12507
C	0.60148	-1.33911	0.75871	C	-0.95404	-0.94317	-0.71780
C	1.92607	-1.27940	0.57398	C	-2.28609	-0.87232	-0.65484
Si	2.93275	0.17352	-0.07981	C	-3.24810	-0.17553	1.53959
C	2.57501	0.46331	-1.90829	C	-2.65923	1.59176	-0.14985
C	2.57033	1.74550	0.89820	C	-4.57644	0.06151	-0.56577
C	4.74897	-0.27470	0.12979	H	5.63684	-1.04422	0.16278
H	-5.83850	-0.76181	-0.89286	C	5.25851	1.06150	-0.34857
C	-5.54991	0.90831	0.50939	H	3.45238	-1.75411	0.71191
H	-3.59154	-1.28442	-1.40651	H	2.46547	1.02415	-0.18608
H	-2.76339	0.78009	0.72278	H	2.09581	0.40132	1.43573
H	-2.18385	0.92480	-0.95015	H	0.14800	0.91587	-0.71816
H	-0.54252	0.34458	1.43681	H	-0.19688	0.27979	0.90472
H	0.03108	0.49012	-0.23993	H	-0.50254	-1.77360	-1.25758
H	0.12801	-2.24154	1.14815	H	-2.83061	-1.67754	-1.14900
H	2.48532	-2.17784	0.84345	H	-2.26131	-0.12229	2.01043
H	1.51964	0.68694	-2.09142	H	-3.64017	-1.18573	1.69495
H	2.83287	-0.42373	-2.49503	H	-3.91095	0.53264	2.05072
H	3.16809	1.30378	-2.28493	H	-1.72046	1.77342	0.37942
H	1.54066	2.08995	0.76070	H	-3.39620	2.30044	0.24412
H	3.23669	2.55410	0.57859	H	-2.50445	1.81439	-1.21086
H	2.72940	1.58031	1.96856	H	-4.98925	-0.94580	-0.44427
H	4.99456	-1.18441	-0.42794	H	-4.55745	0.29430	-1.63606
H	4.99229	-0.44980	1.18286	H	-5.25454	0.76746	-0.07464
H	5.39718	0.52806	-0.23618	H	4.41536	1.73881	-0.49639
H	-4.74066	1.40711	1.04598	H	5.82080	1.00686	-1.28633
H	-6.24558	0.49527	1.24678	H	5.92344	1.51328	0.39577
H	-6.09794	1.67275	-0.05238	C	-3.16791	0.15482	0.03904
Electronic Energy = -757.561677 Zero-point corrected electronic energy=-757.283595 Zero-point corrected Gibbs free energy=-757.330823				Electronic Energy = -506.164731 Zero-point corrected electronic energy=-505.875136 Zero-point corrected Gibbs free energy=-505.919714			
Lithiated Intermediates							
5aA-C^{1}Li				5aCA-C^{1}Li			
C	5.14902	-0.13274	0.15330	C	4.53296	-0.01888	0.60662
C	3.96678	-0.70974	0.37703	C	3.76433	-1.07091	0.30943
C	2.62111	-0.04892	0.31420	C	2.38558	-1.15407	-0.27541

O	1.67145	-1.01945	-0.07464	O	1.82866	0.10611	-0.58563
C	0.36525	-0.54574	-0.07308	C	0.55135	0.01656	-1.14500
C	-0.47520	-0.89453	-1.11221	C	-0.56635	0.00030	-0.30267
C	-1.83314	-0.51431	-1.28213	C	-1.90526	0.06620	-0.70393
Si	-2.93137	0.09456	0.05964	C	-2.78325	0.62128	1.60206
C	-3.03968	-1.01886	1.57980	C	-4.26743	0.78496	-0.39361
C	-2.27024	1.78871	0.71299	C	-3.54154	-1.45324	0.43853
C	-4.65282	0.43503	-0.61886	H	5.50975	-0.25309	1.03135
H	6.03856	-0.75243	0.25584	C	4.25624	1.44968	0.44687
C	5.39839	1.30152	-0.21674	H	4.17833	-2.05845	0.51573
H	3.92887	-1.76214	0.65113	H	1.72373	-1.68341	0.43138
H	2.60491	0.79146	-0.39815	H	2.42303	-1.77501	-1.18730
H	2.34817	0.35614	1.30473	H	0.51828	-0.47104	-2.12654
H	-0.01021	-0.26224	0.91653	H	-0.33690	0.19815	0.74805
H	0.03275	-1.39151	-1.94192	H	-2.12665	-0.29533	-1.71989
H	-2.30791	-0.85477	-2.19859	H	-2.41836	1.65002	1.49921
H	-2.04341	-1.29591	1.93933	H	-2.02666	0.04247	2.14181
H	-3.56331	-1.94538	1.32417	H	-3.68529	0.64076	2.22352
H	-3.57874	-0.53462	2.40133	H	-4.02039	1.84914	-0.48340
H	-1.28904	1.74936	1.20637	H	-5.17639	0.69320	0.21278
H	-2.96156	2.15716	1.47815	H	-4.49237	0.40289	-1.39644
H	-2.25420	2.57298	-0.06121	H	-2.73136	-2.03672	0.88801
H	-5.10527	-0.48874	-0.99352	H	-3.79646	-1.91715	-0.52085
H	-4.61363	1.14825	-1.44849	H	-4.42080	-1.51692	1.09197
H	-5.31158	0.84396	0.15396	H	3.27431	1.63694	0.01858
H	4.47432	1.85401	-0.40005	H	5.01980	1.90478	-0.19457
H	6.01995	1.36587	-1.11586	H	4.32567	1.94880	1.42038
H	5.94088	1.81677	0.58368	C	-3.09949	0.00846	0.23317
Li	-0.68626	1.16702	-0.96705	Li	-0.77780	1.56308	-1.60168
Electronic Energy = -764.4885655 Zero-point corrected electronic energy=-764.222061 Zero-point corrected Gibbs free energy=-764.269983				Electronic Energy = -513.0766782 Zero-point corrected electronic energy=-512.79968 Zero-point corrected Gibbs free energy=-512.845836			
5aA-C^2Li				5aCA-C^2Li			
C	4.69165	0.16903	-0.51740	C	4.74554	-0.13886	-0.18755
C	3.42533	0.74833	-0.56743	C	3.52546	-0.79924	-0.04273
C	2.26928	0.16258	-0.03413	C	2.31317	-0.16405	0.24749
O	1.07921	0.88671	-0.16945	O	1.17646	-0.97145	0.33404
C	-0.28321	-0.56631	1.25384	C	-1.12528	-1.31460	-0.01118
C	-1.47697	-1.03612	0.86699	C	-2.43965	-1.07769	0.01906
Si	-2.77129	-0.13436	-0.17296	C	-3.08214	0.92405	1.37066
C	-3.54426	1.29604	0.78595	C	-2.62560	1.20073	-1.08787
C	-2.00281	0.48601	-1.77374	C	-4.65432	-0.02268	-0.32548
C	-4.12475	-1.38781	-0.55717	H	5.64244	-0.69637	-0.42296
H	5.54594	0.68415	-0.93650	C	4.87150	1.28091	0.29700
C	4.81583	-1.29014	-0.16790	H	3.45583	-1.84481	-0.34540
H	3.33547	1.79066	-0.87595	H	2.28979	0.71656	0.89699
H	0.39892	-1.20981	1.81323	H	-0.78369	-2.34728	0.03576

H	-1.70513	-2.06747	1.14826	H	-3.08413	-1.95365	0.10028
H	-2.82807	2.09861	0.98562	H	-2.04268	1.13733	1.63775
H	-3.93907	0.95087	1.74671	H	-3.50082	0.27401	2.14542
H	-4.37439	1.72475	0.21367	H	-3.63912	1.86845	1.37537
H	-1.11727	1.10177	-1.58747	H	-1.60867	1.53302	-0.86460
H	-2.72640	1.07186	-2.35101	H	-3.25584	2.09502	-1.15444
H	-1.68224	-0.36075	-2.38930	H	-2.61869	0.71245	-2.06817
H	-4.58726	-1.76246	0.36212	H	-5.09459	-0.69117	0.42246
H	-3.72276	-2.24574	-1.10619	H	-4.76281	-0.49472	-1.30824
H	-4.91279	-0.93744	-1.16956	H	-5.22955	0.90917	-0.32852
H	4.41176	-1.56108	0.84178	H	4.17179	2.00198	-0.19893
H	5.85439	-1.62524	-0.17838	H	5.87609	1.67775	0.14094
H	4.23091	-1.93585	-0.84056	H	4.61313	1.38932	1.36191
C	0.22793	0.82387	0.95762	C	-3.17692	0.25384	-0.01092
H	0.76371	1.21468	1.84002	Li	3.34766	0.67782	-1.44885
H	-0.60538	1.49790	0.73582	C	0.00655	-0.32995	-0.11473
Li	3.89746	0.28256	1.37069	H	-0.18327	0.57375	0.48609
H	2.14355	-0.92270	-0.06697	H	0.15019	0.00255	-1.15995
Electronic Energy = -764.4838666 Zero-point corrected electronic energy=-764.216626 Zero-point corrected Gibbs free energy=-764.260906				Electronic Energy = -513.0780418 Zero-point corrected electronic energy=-512.799953 Zero-point corrected Gibbs free energy=-512.843105			
Anionic Intermediates							
5aA-C[1]_anion				5aCA-C[1]_anion			
C	5.12876	0.02815	0.05490	C	4.80432	-0.06435	-0.07564
C	4.00255	-0.67620	0.18883	C	3.64930	-0.72941	0.00456
C	2.60046	-0.13008	0.10542	C	2.27724	-0.11854	0.14116
O	1.69645	-1.20141	0.22581	O	1.32756	-1.15417	0.17113
C	0.34791	-0.78709	0.20442	C	-0.00568	-0.68851	0.30504
C	-0.38989	-0.89424	-0.94064	C	-0.78183	-0.55645	-0.83283
C	-1.74599	-0.56728	-1.21195	C	-2.10448	-0.17682	-1.07450
Si	-2.89335	0.18257	-0.04212	C	-3.34945	-0.91134	0.99376
C	-3.28991	-0.86234	1.51304	C	-2.60503	1.47518	0.76324
C	-2.32499	1.86409	0.67415	C	-4.43532	0.58735	-0.66763
C	-4.57715	0.51654	-0.87214	H	5.73094	-0.62949	-0.17529
H	6.08396	-0.48957	0.13852	C	4.93696	1.43386	-0.04096
C	5.19227	1.50860	-0.20309	H	3.64711	-1.81782	-0.03054
H	4.05115	-1.74749	0.37694	H	2.06309	0.56597	-0.69751
H	2.43389	0.39655	-0.84936	H	2.21193	0.48645	1.06372
H	2.42423	0.60879	0.90774	H	-0.30903	-0.52996	1.33590
H	-0.01695	-0.41955	1.16328	H	-0.21914	-0.82371	-1.73463
H	0.19047	-1.31576	-1.77110	H	-2.45542	-0.18627	-2.10352
H	-2.10182	-0.78587	-2.21757	H	-2.40277	-1.27994	1.40194
H	-2.36305	-1.18011	2.00451	H	-3.83351	-1.74997	0.48040
H	-3.83298	-1.76922	1.22290	H	-3.99202	-0.59104	1.82902
H	-3.89571	-0.31000	2.24379	H	-1.59865	1.30517	1.16033
H	-1.31682	1.77405	1.09505	H	-3.27470	1.73068	1.59941
H	-2.99589	2.23100	1.46182	H	-2.54896	2.33296	0.08321

H	-2.28015	2.61321	-0.12482
H	-5.00517	-0.41401	-1.26257
H	-4.46257	1.21346	-1.71020
H	-5.29121	0.94957	-0.16095
H	4.19494	1.94247	-0.30908
H	5.75349	1.72631	-1.11944
H	5.70134	2.03050	0.61611

Electronic Energy = -756.9580354
Zero-point corrected electronic energy=-756.696904
Zero-point corrected Gibbs free energy=-756.746337

H	-4.82667	-0.27674	-1.21958
H	-4.30320	1.41188	-1.37960
H	-5.18155	0.88869	0.08100
H	3.96399	1.92011	0.06465
H	5.40402	1.81100	-0.95875
H	5.56831	1.75608	0.79598
C	-3.09674	0.23391	-0.01038

Electronic Energy = -505.5446257
Zero-point corrected electronic energy=-505.272789
Zero-point corrected Gibbs free energy=-505.317141

5aA-C^2_anion

C	5.06090	-0.02583	-0.40375
C	3.81192	-0.61233	-0.27505
C	2.67142	-0.08656	0.32621
O	1.57211	-0.96561	0.54689
C	-0.65220	-1.61547	0.09729
C	-1.97750	-1.40416	0.12867
Si	-2.83314	0.25291	-0.03802
C	-2.55989	1.33983	1.48111
C	-2.28908	1.18871	-1.58297
C	-4.69038	-0.08654	-0.18049
H	5.83858	-0.51259	-0.98321
C	5.27737	1.35958	0.11892
H	3.67057	-1.60608	-0.71165
H	2.68361	0.76703	1.00265
H	-0.24741	-2.62316	0.21135
H	-2.61434	-2.28317	0.25722
H	-1.49548	1.52714	1.65035
H	-2.96053	0.85468	2.37715
H	-3.06193	2.30655	1.36069
H	-1.22658	1.44767	-1.54410
H	-2.86319	2.11635	-1.69133
H	-2.45115	0.57966	-2.47858
H	-5.05801	-0.62247	0.70167
H	-4.91164	-0.69810	-1.06192
H	-5.25570	0.84793	-0.26693
H	4.57909	2.09222	-0.33740
H	6.29857	1.71847	-0.06114
H	5.09207	1.43167	1.20817
C	0.41134	-0.57474	-0.12485
H	0.06957	0.41695	0.22097
H	0.61769	-0.47165	-1.20729

Electronic Energy = -756.9382848
Zero-point corrected electronic energy=-756.677396
Zero-point corrected Gibbs free energy=-

5aCA-C^2_anion

C	4.74433	-0.06981	-0.56006
C	3.46251	-0.57780	-0.40621
C	2.44058	-0.10808	0.41163
O	1.27433	-0.90796	0.56197
C	-1.01451	-1.29413	0.16433
C	-2.33202	-1.06481	0.13289
C	-2.97456	1.10153	1.21430
C	-2.49481	1.05446	-1.25283
C	-4.53936	-0.04607	-0.35715
H	5.41747	-0.48984	-1.30016
C	5.13814	1.16077	0.19445
H	3.18933	-1.45294	-1.00474
H	2.58082	0.61411	1.21358
H	-0.67714	-2.31512	0.34205
H	-2.98530	-1.92426	0.29649
H	-1.93414	1.32628	1.46484
H	-3.41625	0.56283	2.05972
H	-3.51328	2.04964	1.08849
H	-1.46514	1.37279	-1.07628
H	-3.10022	1.95367	-1.42444
H	-2.50826	0.44987	-2.16606
H	-4.99285	-0.60450	0.47024
H	-4.64122	-0.64672	-1.26852
H	-5.10689	0.88200	-0.49355
H	4.47486	2.02236	-0.03207
H	6.16845	1.47055	-0.02229
H	5.06057	1.02464	1.29105
C	-3.06184	0.25709	-0.06878
C	0.13415	-0.33504	-0.01919
H	-0.07706	0.64583	0.43827
H	0.31596	-0.14601	-1.09265

Electronic Energy = -505.5396598
Zero-point corrected electronic energy=-505.267273
Zero-point corrected Gibbs free energy=-

756.724753				505.310691			
5b_Reactant				5bC_Reactant			
C	-4.94435	0.17766	0.29459	C	-4.67110	-0.25402	-0.28163
C	-3.78068	0.28632	-0.34551	C	-3.55157	-0.07409	0.41844
C	-2.47008	0.51278	0.33951	C	-2.22653	-0.65612	0.03905
O	-1.56458	-0.49877	-0.05669	O	-1.26699	0.38038	-0.00737
C	-0.28120	-0.32345	0.50099	C	0.02829	-0.09758	-0.30013
C	0.58867	-1.46290	0.05505	C	0.95300	1.08678	-0.33670
C	1.90269	-1.39015	-0.19050	C	2.28107	1.11008	-0.19744
Si	3.01236	0.12886	-0.07977	C	3.15076	-0.47958	1.52693
C	2.61652	1.34705	-1.46322	C	2.96106	-1.24228	-0.86497
C	2.82910	0.98285	1.59255	C	4.66798	0.45174	-0.22579
C	4.78758	-0.46742	-0.27275	C	-6.01493	0.29345	0.09663
C	-6.27307	-0.02161	-0.37146	H	-4.62472	-0.84063	-1.20060
H	-4.94847	0.23503	1.38433	H	-3.56451	0.51924	1.33267
H	-3.74298	0.21820	-1.43273	H	-2.29435	-1.16244	-0.93750
H	-2.60116	0.50311	1.43368	H	-1.91122	-1.40752	0.78367
H	-2.05695	1.49741	0.06032	H	0.01990	-0.61648	-1.27502
H	-0.35369	-0.31354	1.60370	H	0.33621	-0.83322	0.45982
H	0.14007	0.64667	0.19106	H	0.43087	2.02712	-0.50406
H	0.05092	-2.40757	-0.03746	H	2.75108	2.09243	-0.25305
H	2.38622	-2.32707	-0.47522	H	2.14670	-0.83556	1.77693
H	1.58531	1.70925	-1.40927	H	3.38524	0.35679	2.19299
H	2.75202	0.87530	-2.44134	H	3.86137	-1.28969	1.72833
H	3.28186	2.21557	-1.41019	H	2.00568	-1.72385	-0.64115
H	1.83443	1.41889	1.72775	H	3.74463	-1.99812	-0.74016
H	3.56212	1.79118	1.68846	H	2.94920	-0.93202	-1.91506
H	2.99949	0.27470	2.40979	H	4.91849	1.30505	0.41385
H	4.93012	-0.96843	-1.23590	H	4.77336	0.76722	-1.26968
H	5.05287	-1.17646	0.51828	H	5.39720	-0.34236	-0.03385
H	5.49069	0.37032	-0.22320	H	-5.95831	0.87370	1.02119
H	-6.16457	-0.08066	-1.45749	H	-6.74184	-0.51288	0.24091
H	-6.95699	0.80127	-0.13791	H	-6.40776	0.94197	-0.69351
H	-6.74873	-0.94391	-0.02181	C	3.24174	-0.04369	0.05432
Electronic Energy =-757.5640534 Zero-point corrected electronic energy=-757.286012 Zero-point corrected Gibbs free energy=-757.332763				Electronic Energy = -506.167088 Zero-point corrected electronic energy=-505.877449 Zero-point corrected Gibbs free energy=-505.920296			
Lithiated Intermediates							
5bA-C^{1}Li				5bCA-C^{1}Li			
C	-3.62478	-0.19257	0.10886	C	4.65895	0.24073	-0.38584
C	-2.40499	-0.04132	-0.40803	C	3.63789	0.09712	0.45844
C	-1.73927	1.28559	-0.58332	C	2.25132	0.59235	0.18674

O	-0.57569	1.32909	0.23747	O	1.34145	-0.47693	0.32309
C	0.30013	2.41794	0.01296	C	0.00484	-0.07714	0.20204
C	1.63498	2.17617	0.18337	C	-0.84911	-0.95032	-0.47685
C	2.25514	0.93379	0.53825	C	-2.21335	-0.82446	-0.76810
Si	1.76351	-0.74463	-0.04659	C	-3.23140	-0.38335	1.50561
C	3.30338	-1.84012	-0.02319	C	-2.93382	1.53635	-0.07707
C	0.52134	-1.63553	1.10405	C	-4.61118	-0.21859	-0.57021
C	1.03980	-0.75447	-1.79620	C	6.06241	-0.21814	-0.12167
C	-4.32243	-1.50742	0.28474	H	4.47759	0.72576	-1.34655
H	-4.16999	0.69787	0.42706	H	3.78662	-0.39888	1.41783
H	-1.83099	-0.91099	-0.72985	H	2.18413	1.02513	-0.82634
H	-2.41584	2.10523	-0.30120	H	1.98834	1.39018	0.90282
H	-1.42292	1.44059	-1.62388	H	-0.33913	0.54509	1.03326
H	-0.16775	3.37752	-0.17128	H	-0.31556	-1.73113	-1.02311
H	2.25014	3.07577	0.15188	H	-2.64596	-1.62131	-1.36572
H	3.76006	-1.84304	0.97265	H	-2.24205	-0.27103	1.95963
H	4.05071	-1.47385	-0.73439	H	-3.52025	-1.43438	1.59916
H	3.06071	-2.87543	-0.28577	H	-3.94427	0.22538	2.07617
H	-0.41694	-1.08871	1.26236	H	-1.95496	1.81784	0.33618
H	0.24371	-2.61248	0.68844	H	-3.67130	2.11155	0.49206
H	0.98631	-1.82213	2.08034	H	-3.01729	1.88702	-1.11990
H	1.83692	-0.58279	-2.52727	H	-4.87853	-1.27784	-0.49845
H	0.30791	0.04984	-1.92248	H	-4.63768	0.06409	-1.62913
H	0.55399	-1.70634	-2.03953	H	-5.37099	0.36274	-0.03565
H	-3.69058	-2.33606	-0.04466	H	6.14167	-0.69912	0.85677
H	-5.25510	-1.53439	-0.28838	H	6.76354	0.62310	-0.14841
H	-4.58666	-1.67038	1.33484	H	6.39007	-0.93320	-0.88380
Li	0.57413	1.14285	1.74406	C	-3.21704	0.01919	0.02015
H	3.32057	1.02103	0.74236	Li	-1.09419	0.84066	-1.40696
Electronic Energy = -764.5049627 Zero-point corrected electronic energy=-764.237395 Zero-point corrected Gibbs free energy=-764.282429				Electronic Energy = -513.0814238 Zero-point corrected electronic energy=-512.803592 Zero-point corrected Gibbs free energy=-512.846709			
5bA-C^2Li				5bCA-C^2Li			
C	-3.04195	1.22086	-0.68254	C	4.63256	0.46562	0.16461
C	-2.78937	-0.14497	-0.55124	C	3.44279	-0.25664	0.07097
C	-2.19128	-0.74585	0.55694	C	2.17892	0.14922	0.52206
O	-1.74663	-2.08148	0.44484	O	1.11991	-0.74858	0.34957
C	0.04464	-1.47940	-1.05048	C	-1.11953	-1.20928	-0.20123
C	0.95793	-0.50821	-1.23746	C	-2.45057	-1.09652	-0.21090
Si	2.08681	0.34647	0.01566	C	-3.35434	0.54919	1.43940
C	1.06281	1.57912	1.03019	C	-2.79958	1.32582	-0.88842
C	2.95896	-0.84810	1.17398	C	-4.73593	-0.18919	-0.50791
C	3.35238	1.31003	-0.98427	C	5.94405	-0.06668	-0.35967
C	-3.01485	2.09440	0.54720	H	4.70489	1.21158	0.96556
H	-3.53302	1.59226	-1.57336	H	3.43159	-1.12541	-0.59362
H	-2.86429	-0.76477	-1.44691	H	2.10467	0.75259	1.43637
H	-2.37143	-0.41816	1.57964	H	-0.68273	-2.19918	-0.32212

H	-0.51077	-1.86140	-1.91044	H	-3.01040	-2.02476	-0.33051
H	1.10004	-0.19107	-2.27458	H	-2.35508	0.78982	1.81498
H	0.30465	1.08604	1.65134	H	-3.75362	-0.26732	2.04945
H	0.58139	2.34502	0.40395	H	-3.99543	1.42790	1.57832
H	1.71849	2.12899	1.71379	H	-1.83699	1.70149	-0.53247
H	2.27845	-1.29212	1.90546	H	-3.51383	2.15589	-0.84002
H	3.74748	-0.32363	1.72418	H	-2.68635	1.03216	-1.93740
H	3.42608	-1.66106	0.60949	H	-5.14857	-1.02211	0.07189
H	2.86516	2.00768	-1.67354	H	-4.74499	-0.47452	-1.56567
H	3.97922	0.63658	-1.57747	H	-5.39841	0.67368	-0.38051
H	4.00898	1.89041	-0.32839	H	5.76985	-0.77137	-1.18033
H	-2.05351	2.03914	1.10335	H	6.52043	-0.60119	0.40748
H	-3.76433	1.79606	1.29711	H	6.58993	0.72829	-0.74738
H	-3.17827	3.14616	0.30208	C	-3.31112	0.14796	-0.04515
Li	-1.00193	0.82876	-0.30618	Li	3.09359	1.61492	-0.67024
C	-0.35067	-2.13884	0.25102	C	-0.08208	-0.13103	-0.04693
H	0.17557	-1.67364	1.09835	H	-0.38552	0.62035	0.69944
H	-0.07794	-3.20171	0.21649	H	0.07945	0.40513	-1.00028
Electronic Energy = -764.487529				Electronic Energy = -513.0723401			
Zero-point corrected electronic energy=-764.220388				Zero-point corrected electronic energy=-512.795256			
Zero-point corrected Gibbs free energy=-764.264759				Zero-point corrected Gibbs free energy=-512.839437			
Anionic Intermediates							
5bA-C^1_anion				5bCA-C^1_anion			
C	4.92206	0.25489	0.47960	C	-4.52545	0.53583	-0.21199
C	3.91156	-0.42492	-0.06253	C	-3.57415	-0.39699	-0.16059
C	2.47249	-0.29085	0.34148	C	-2.13195	-0.17544	-0.51624
O	1.68634	-0.10018	-0.81118	O	-1.31983	-0.67192	0.51979
C	0.30096	-0.11188	-0.53786	C	0.06750	-0.58610	0.22932
C	-0.39139	1.05967	-0.41930	C	0.77433	0.51727	0.67248
C	-1.76953	1.30967	-0.17520	C	2.11251	0.91428	0.60154
Si	-3.02654	0.04734	0.08990	C	3.40476	-1.25255	0.62454
C	-3.29190	-1.16666	-1.36680	C	2.93151	-0.10230	-1.55685
C	-2.71412	-1.10874	1.58429	C	4.53901	0.88870	0.06013
C	-4.73087	0.84383	0.40283	C	-5.97329	0.30816	0.12007
C	6.36611	0.09991	0.09469	H	-4.24647	1.54866	-0.50765
H	4.70058	0.98718	1.25780	H	-3.82731	-1.40974	0.15994
H	4.10850	-1.14348	-0.86043	H	-1.93580	0.89518	-0.69056
H	2.34122	0.54504	1.04754	H	-1.89550	-0.70315	-1.45790
H	2.14694	-1.20850	0.86306	H	0.45513	-1.45469	-0.29498
H	-0.12569	-1.11213	-0.46398	H	0.12448	1.22284	1.20306
H	0.25275	1.93842	-0.54934	H	2.38969	1.85249	1.07584
H	-2.07249	2.35532	-0.15190	H	2.45280	-1.79196	0.66815
H	-2.33410	-1.59506	-1.68368	H	3.74655	-1.10673	1.65563
H	-3.71004	-0.63125	-2.22719	H	4.14010	-1.87825	0.09425
H	-3.96897	-1.99032	-1.10440	H	1.93930	-0.54363	-1.69691
H	-1.71217	-1.54896	1.51860	H	3.67962	-0.76222	-2.02352
H	-3.44599	-1.92533	1.63891	H	2.93892	0.86156	-2.07871

H	-2.75888	-0.53515	2.51726
H	-5.02731	1.46409	-0.45089
H	-4.70369	1.48331	1.29246
H	-5.50248	0.07893	0.55399
H	6.48095	-0.64798	-0.69547
H	6.97708	-0.21163	0.95019
H	6.78243	1.04659	-0.26891

Electronic Energy = -756.9594476
Zero-point corrected electronic energy=-756.698064
Zero-point corrected Gibbs free energy=-756.745684

H	4.78800	1.05812	1.11545
H	4.45224	1.86788	-0.42776
H	5.36626	0.33765	-0.40887
H	-6.14692	-0.73155	0.41359
H	-6.62144	0.53313	-0.73552
H	-6.29694	0.95325	0.94544
C	3.21786	0.12022	-0.05695

Electronic Energy = -505.5458137
Zero-point corrected electronic energy=-505.27398
Zero-point corrected Gibbs free energy=-505.317918

5bA-C^2_anion

C	5.04737	-0.54502	-0.17144
C	3.79838	0.03231	-0.05407
C	2.52957	-0.41950	-0.43993
O	1.53085	0.59560	-0.61096
C	-0.59968	1.46252	-0.08987
C	-1.94150	1.40893	-0.06521
Si	-2.97628	-0.14318	0.07955
C	-2.92368	-1.16615	-1.50797
C	-2.45543	-1.22382	1.53536
C	-4.76896	0.39845	0.35955
C	6.25130	-0.03393	0.56975
H	5.14522	-1.50661	-0.67765
H	3.76926	1.00095	0.46335
H	2.42193	-1.22537	-1.17160
H	-0.08445	2.42063	-0.18497
H	-2.47475	2.36059	-0.13155
H	-1.90161	-1.47822	-1.74233
H	-3.29593	-0.57904	-2.35393
H	-3.54398	-2.06478	-1.41355
H	-1.43936	-1.60887	1.40678
H	-3.13465	-2.07775	1.64237
H	-2.47773	-0.64993	2.46769
H	-5.11690	1.03536	-0.46134
H	-4.86481	0.96754	1.29064
H	-5.43766	-0.46715	0.42157
H	6.06808	0.99055	0.92374
H	7.15978	0.00553	-0.05327
H	6.52812	-0.62280	1.46690
C	0.34149	0.29742	0.04965
H	-0.11703	-0.62446	-0.35355
H	0.54435	0.09634	1.11998

Electronic Energy = -756.9321211
Zero-point corrected electronic energy=-756.67161
Zero-point corrected Gibbs free energy=-

5bCA-C^2_anion

C	-4.80504	-0.44919	0.12994
C	-3.51508	0.04149	0.04967
C	-2.28876	-0.51399	0.43180
O	-1.22364	0.41545	0.66310
C	0.97687	1.13589	0.26003
C	2.31196	1.09566	0.18030
C	3.27327	-1.03233	1.09115
C	2.72546	-0.87997	-1.35707
C	4.62394	0.42720	-0.41761
C	-5.95429	0.16776	-0.61775
H	-4.97656	-1.42244	0.59270
H	-3.40972	1.02724	-0.42375
H	-2.24766	-1.36514	1.11814
H	0.50873	2.08712	0.51271
H	2.84542	2.02629	0.38369
H	2.28103	-1.41885	1.33961
H	3.65528	-0.49737	1.96743
H	3.93663	-1.88330	0.88846
H	1.75513	-1.35130	-1.18605
H	3.44590	-1.66977	-1.60596
H	2.62764	-0.21600	-2.22270
H	5.01519	0.98942	0.43860
H	4.62056	1.09369	-1.28788
H	5.31076	-0.40220	-0.62354
H	-5.70490	1.19895	-0.90629
H	-6.87911	0.22296	-0.02054
H	-6.23377	-0.35291	-1.55610
C	3.20974	-0.09592	-0.12786
C	-0.03608	0.04353	0.03061
H	0.32412	-0.92558	0.41826
H	-0.21748	-0.10519	-1.05087

Electronic Energy = -505.5333752
Zero-point corrected electronic energy=-505.261304
Zero-point corrected Gibbs free energy=-

756.71941				505.304968			
6a_Reactant				6aC_Reactant			
C	-5.50116	0.25747	-0.61389	C	5.34685	0.24268	-0.36859
C	-4.40913	0.33385	-0.10959	C	4.23535	-0.15753	-0.13000
C	-3.09364	0.44776	0.52330	C	2.89715	-0.67579	0.16218
O	-2.20636	-0.48580	-0.04899	O	1.95557	0.36995	0.09919
C	-0.93068	-0.43769	0.55891	C	0.64847	-0.08262	0.39546
C	-0.06906	-1.48896	-0.07518	C	-0.26840	1.10336	0.29424
C	1.23351	-1.35994	-0.35499	C	-1.58922	1.11648	0.09834
Si	2.33243	0.14892	-0.08412	C	-2.39080	-0.62579	-1.50971
C	1.80998	1.56777	-1.21043	C	-2.31880	-1.15938	0.95030
C	2.27896	0.70878	1.71635	C	-3.97971	0.47393	0.07365
C	4.09001	-0.36784	-0.51579	H	2.89453	-1.13508	1.16351
H	-3.19305	0.26815	1.60551	H	2.64540	-1.46414	-0.56465
H	-2.71168	1.47212	0.39048	H	0.62814	-0.51084	1.41287
H	-1.03113	-0.63349	1.64150	H	0.36233	-0.88194	-0.30564
H	-0.49104	0.56514	0.44225	H	0.25302	2.05270	0.40107
H	-0.59989	-2.41915	-0.28209	H	-2.05441	2.10133	0.04810
H	1.71456	-2.24020	-0.78677	H	-1.38317	-1.01893	-1.67575
H	0.79225	1.91118	-1.00124	H	-2.57679	0.14651	-2.26252
H	1.84668	1.25883	-2.25957	H	-3.10567	-1.44129	-1.66941
H	2.48518	2.42103	-1.08385	H	-1.35451	-1.65796	0.82286
H	1.28574	1.06151	2.01136	H	-3.09681	-1.92505	0.85452
H	2.98563	1.52945	1.88077	H	-2.36185	-0.75266	1.96599
H	2.55492	-0.11277	2.38505	H	-4.19269	1.26043	-0.65853
H	4.15503	-0.70587	-1.55525	H	-4.12983	0.89207	1.07501
H	4.42805	-1.18775	0.12625	H	-4.70645	-0.33187	-0.07255
H	4.78738	0.46660	-0.39026	H	6.32688	0.60783	-0.58058
H	-6.46439	0.17963	-1.06673	C	-2.54634	-0.05213	-0.09049
Electronic Energy = -717.0143614 Zero-point corrected electronic energy=-716.788865 Zero-point corrected Gibbs free energy=-716.833753				Electronic Energy = -465.6175042 Zero-point corrected electronic energy=-465.379948 Zero-point corrected Gibbs free energy=-465.419853			
Lithiated Intermediates							
6aA-C[1]Li				6aCA-C[1]Li			
C	-5.71734	0.10091	-0.21066	C	-5.44543	-0.18823	-0.16093
C	-4.54867	0.26903	0.03299	C	-4.29890	0.16470	-0.03902
C	-3.13634	0.49581	0.35445	C	-2.91522	0.62427	0.12529
O	-2.32987	-0.41616	-0.35339	O	-2.02306	-0.41125	-0.20232
C	-0.96919	-0.22158	-0.11834	C	-0.67984	-0.01506	-0.08769
C	-0.16293	-1.33713	0.02931	C	0.19718	-0.98756	0.41564
C	1.23523	-1.35561	0.25246	C	1.57363	-0.91812	0.63250
Si	2.37946	0.04478	-0.08979	C	2.46385	-0.16333	-1.60827
C	2.28460	0.74765	-1.83739	C	2.29388	1.51057	0.24929

C	1.95482	1.51772	1.08564	C	3.96738	-0.31319	0.38122
C	4.14630	-0.45446	0.31911	H	-2.75442	0.95126	1.16596
H	-2.97980	0.37794	1.43907	H	-2.74765	1.50007	-0.52112
H	-2.86863	1.53141	0.09313	H	-0.37153	0.68276	-0.87221
H	-0.58187	0.73225	-0.49281	H	-0.31892	-1.82818	0.88426
H	-0.71805	-2.27309	0.12703	H	2.02617	-1.78389	1.10665
H	1.67862	-2.33712	0.39885	H	1.45327	0.03132	-1.97992
H	1.24926	0.95590	-2.12564	H	2.71840	-1.19475	-1.86865
H	2.68222	0.02046	-2.55205	H	3.15846	0.50858	-2.12779
H	2.86031	1.67456	-1.93365	H	1.29520	1.85618	-0.05490
H	0.95986	1.96282	0.94379	H	3.00185	2.15690	-0.27916
H	2.66058	2.33125	0.88807	H	2.44979	1.70691	1.32362
H	2.09207	1.26891	2.15017	H	4.21219	-1.35160	0.13543
H	4.47068	-1.27651	-0.32682	H	4.06184	-0.19325	1.46684
H	4.22780	-0.79288	1.35705	H	4.70411	0.33617	-0.10494
H	4.83938	0.38070	0.17567	H	-6.45509	-0.51328	-0.27572
H	-6.74823	-0.05741	-0.43612	C	2.54581	0.02179	-0.08290
Li	0.32777	-0.12362	1.64436	Li	0.51226	0.66994	1.55649
Electronic Energy = -723.9420069 Zero-point corrected electronic energy=-723.727127 Zero-point corrected Gibbs free energy=-723.770355				Electronic Energy = -472.5331619 Zero-point corrected electronic energy=-472.307328 Zero-point corrected Gibbs free energy=-472.347335			
6aA-C^2Li				6aCA-C^2Li			
C	-5.51362	0.09668	0.11350	C	5.23373	0.05821	-0.29204
C	-4.32310	0.22613	-0.35541	C	4.09853	0.00558	0.31080
C	-2.99946	0.47846	-0.39131	C	2.80628	0.26076	0.59542
O	-2.08688	-0.57924	-0.39281	O	1.81562	-0.64459	0.21043
C	0.03458	-1.44631	0.17145	C	-0.40169	-1.09199	-0.42945
C	1.36998	-1.40430	0.08746	C	-1.73619	-1.03942	-0.41548
Si	2.46725	0.12449	-0.00603	C	-2.69438	0.20377	1.52949
C	2.25588	0.99541	-1.66430	C	-2.20200	1.45048	-0.60086
C	2.07769	1.32604	1.39630	C	-4.06296	-0.19933	-0.52204
C	4.24925	-0.45660	0.16842	H	2.51834	0.94769	1.39207
H	-2.60649	1.42538	-0.76308	H	0.08023	-2.01638	-0.74289
H	-0.49681	-2.39809	0.21596	H	-2.25487	-1.95025	-0.71616
H	1.87726	-2.37128	0.07571	H	-1.70382	0.41222	1.94540
H	1.22345	1.31794	-1.83010	H	-3.04965	-0.73494	1.96619
H	2.53041	0.32860	-2.48734	H	-3.37284	1.00665	1.84092
H	2.89845	1.88101	-1.71589	H	-1.25790	1.79972	-0.17478
H	1.07197	1.74919	1.31048	H	-2.95634	2.21825	-0.39483
H	2.78997	2.15835	1.39027	H	-2.08073	1.37346	-1.68659
H	2.15194	0.82625	2.36753	H	-4.42997	-1.14916	-0.11825
H	4.51022	-1.16585	-0.62398	H	-4.07305	-0.26886	-1.61540
H	4.40883	-0.95344	1.13096	H	-4.76207	0.58896	-0.22337
H	4.94469	0.38666	0.10586	H	6.13749	-0.47356	-0.01875
C	-0.87354	-0.25297	0.24600	C	-2.64966	0.10687	-0.00546
H	-0.41451	0.63006	-0.22671	C	0.58111	-0.01666	-0.05978
H	-1.07001	0.01121	1.30315	H	0.24867	0.55479	0.82089

Li	-4.30922	0.62191	1.59388	H	0.70600	0.70806	-0.88644
H	-6.40414	-0.17584	-0.44025	Li	3.96296	1.23681	-1.24505
Electronic Energy = -723.9399094 Zero-point corrected electronic energy=-723.725352 Zero-point corrected Gibbs free energy=-723.771673				Electronic Energy = -472.5429906 Zero-point corrected electronic energy=-472.31684 Zero-point corrected Gibbs free energy=-472.358388			
Anionic Intermediates							
6aA-C^1_anion				6aCA-C^1_anion			
C	5.73645	-0.13868	0.02345	C	5.40834	0.08084	0.05282
C	4.54392	-0.20791	0.20437	C	4.22590	-0.11274	0.21202
C	3.09335	-0.30646	0.44704	C	2.78676	-0.36098	0.42449
O	2.37759	0.25973	-0.62383	O	2.03475	0.15820	-0.64419
C	0.98050	0.12663	-0.44847	C	0.64428	-0.08800	-0.48013
C	0.25268	1.15660	0.08121	C	-0.13760	0.89347	0.10651
C	-1.13717	1.28049	0.33655	C	-1.49933	1.01720	0.38346
Si	-2.36454	-0.00985	0.05260	C	-2.62682	-0.28826	-1.45718
C	-2.54843	-0.58416	-1.76327	C	-2.25362	-1.35498	0.78463
C	-2.04969	-1.63163	1.01709	C	-3.92108	0.47271	0.52621
C	-4.09787	0.58284	0.57939	H	2.47705	0.09925	1.37511
H	2.84689	0.20550	1.38939	H	2.62353	-1.44584	0.52556
H	2.82572	-1.36720	0.57659	H	0.31690	-1.02386	-0.92201
H	0.58066	-0.82094	-0.80645	H	0.46303	1.75978	0.40672
H	0.87841	2.02226	0.33266	H	-1.84122	1.93836	0.84875
H	-1.47089	2.23752	0.73426	H	-1.63827	-0.53867	-1.85569
H	-1.57872	-0.90012	-2.16472	H	-2.96685	0.61822	-1.97084
H	-2.90284	0.24732	-2.38325	H	-3.32073	-1.10971	-1.69486
H	-3.25186	-1.42123	-1.86392	H	-1.23288	-1.68981	0.57182
H	-1.01433	-1.96031	0.86919	H	-2.95443	-2.14898	0.48299
H	-2.71794	-2.44410	0.70359	H	-2.33273	-1.21000	1.86821
H	-2.18846	-1.45913	2.09065	H	-4.17550	1.41282	0.02055
H	-4.39557	1.46615	0.00280	H	-3.91085	0.66175	1.60705
H	-4.10560	0.85453	1.64121	H	-4.70760	-0.26326	0.30841
H	-4.85039	-0.19907	0.42024	H	6.44680	0.26339	-0.10357
H	6.78540	-0.06756	-0.15218	C	-2.54754	-0.02409	0.06139
Electronic Energy = -716.4151883 Zero-point corrected electronic energy=-716.205763 Zero-point corrected Gibbs free energy=-716.250213				Electronic Energy = -465.0024048 Zero-point corrected electronic energy=-464.782281 Zero-point corrected Gibbs free energy=-464.822508			
6aA-C^2_anion				6aCA-C^2_anion			
C	2.36182	-2.16289	0.61948	C	3.35726	-2.01055	-0.04489
C	2.62194	-1.07848	-0.02972	C	3.37764	-0.71997	-0.00337
C	2.84616	0.14160	-0.53744	C	3.25046	0.60210	0.17355
O	1.79185	1.09470	-0.62979	O	2.07825	1.30343	-0.23620
C	-0.02854	2.19512	0.42933	C	-0.26722	1.49323	-0.24970
C	-1.20558	1.61590	0.15104	C	-1.54634	1.11452	-0.34874

Si	-1.53144	-0.23476	-0.05422	C	-1.81133	-1.26670	-1.07665
C	-0.68659	-0.90911	-1.58906	C	-1.70086	-0.74292	1.37809
C	-1.05759	-1.24370	1.46459	C	-3.69108	-0.06168	0.04542
C	-3.41374	-0.36991	-0.28357	H	3.98677	1.25866	0.62276
H	3.79622	0.51565	-0.90241	H	-0.00344	2.49903	-0.57685
H	0.04510	3.28462	0.46273	H	-2.24586	1.84390	-0.76196
H	-2.05228	2.28659	-0.02553	H	-0.73002	-1.41687	-1.14043
H	0.39460	-0.74841	-1.51693	H	-2.16787	-0.93370	-2.05772
H	-1.05437	-0.40424	-2.48931	H	-2.27884	-2.23310	-0.84833
H	-0.87380	-1.98488	-1.68691	H	-0.64077	-1.00560	1.38241
H	0.01503	-1.47623	1.47368	H	-2.26595	-1.64326	1.64982
H	-1.60546	-2.19424	1.45281	H	-1.86983	0.01632	2.14974
H	-1.31426	-0.71490	2.38912	H	-4.06956	0.29900	-0.91843
H	-3.75016	0.22199	-1.14263	H	-3.98235	0.66146	0.81657
H	-3.94741	-0.01226	0.60459	H	-4.18104	-1.01669	0.26815
H	-3.70811	-1.41113	-0.45712	H	3.75548	-2.48876	-0.94853
H	1.99759	-3.02544	0.04678	C	-2.16521	-0.23176	0.00545
C	1.25049	1.42410	0.63703	C	0.90895	0.71420	0.27046
H	1.05314	0.50174	1.20212	H	0.86330	-0.34529	-0.02158
H	1.97920	2.01438	1.21638	H	0.93043	0.73456	1.37631
Electronic Energy = -716.4096723 Zero-point corrected electronic energy=-716.198899 Zero-point corrected Gibbs free energy=-716.242093				Electronic Energy = -465.0087222 Zero-point corrected electronic energy=-464.78667 Zero-point corrected Gibbs free energy=-464.826808			
6b_Reactant				6bC_Reactant			
C	5.06526	-1.43442	-0.15109	C	-4.84912	-1.39596	0.12826
C	4.11320	-0.76952	0.17240	C	-3.91266	-0.69886	-0.17208
C	2.97185	0.04477	0.59757	C	-2.79240	0.16077	-0.56394
O	2.09562	0.23209	-0.49166	O	-1.81380	0.14820	0.45102
C	0.83910	0.79199	-0.12692	C	-0.57336	0.73311	0.06122
C	-0.02561	0.70490	-1.35414	C	0.37685	0.43628	1.18830
C	-1.29927	0.29503	-1.37827	C	1.63348	-0.01259	1.13150
Si	-2.32991	-0.35498	0.06193	C	1.91211	-1.67475	-0.73131
C	-1.64474	-2.00154	0.67354	C	2.56154	0.73312	-1.11076
C	-2.38668	0.87944	1.48835	C	3.90092	-0.70122	0.41585
C	-4.07944	-0.61096	-0.58403	H	-3.17196	1.17652	-0.74249
H	3.34461	1.00480	0.98053	H	-2.36631	-0.20801	-1.51075
H	2.45058	-0.46527	1.42344	C	-0.70274	2.24222	-0.15826
C	0.97180	2.24227	0.34208	H	-0.24319	0.25276	-0.87092
H	0.40415	0.18294	0.68278	H	-0.05587	0.63938	2.16774
H	0.47668	1.04319	-2.26274	H	2.13267	-0.14072	2.09266
H	-1.79340	0.33027	-2.35174	H	0.89560	-1.52438	-1.10541
H	-0.62166	-1.90693	1.05068	H	1.88115	-2.49724	-0.01007
H	-1.63115	-2.73636	-0.13725	H	2.54408	-1.97905	-1.57379
H	-2.26739	-2.39871	1.48254	H	1.59498	0.94536	-1.57512
H	-1.41227	1.00572	1.97087	H	3.25891	0.45874	-1.91059
H	-3.09323	0.53595	2.25204	H	2.92352	1.65538	-0.64413
H	-2.72012	1.86251	1.14016	H	3.89654	-1.51055	1.15401

H	-4.09294	-1.32632	-1.41287
H	-4.50641	0.33037	-0.94534
H	-4.73512	-0.99708	0.20306
H	5.90363	-2.02468	-0.44715
H	1.46266	2.83702	-0.43467
H	1.55247	2.32187	1.26595
H	-0.02021	2.66195	0.52899

Electronic Energy = -756.3147231
Zero-point corrected electronic energy=-756.060781
Zero-point corrected Gibbs free energy=-756.106437

H	4.34638	0.18381	0.88350
H	4.54196	-1.00529	-0.41816
H	-5.67290	-2.01572	0.40402
H	-1.10212	2.71071	0.74667
H	-1.36312	2.47900	-0.99777
H	0.27962	2.67342	-0.36775
C	2.47713	-0.40207	-0.07709

Electronic Energy = -504.9168591
Zero-point corrected electronic energy=-504.651248
Zero-point corrected Gibbs free energy=-504.692703

Lithiated Intermediates

6bA-C[1]Li

C	-5.79506	-0.34208	-0.04678
C	-4.63237	-0.09924	-0.25371
C	-3.22709	0.20665	-0.53775
O	-2.42562	-0.16529	0.55861
C	-1.05118	0.04820	0.34568
C	-0.23763	-0.99694	0.75068
C	1.16429	-1.17877	0.61188
Si	2.52129	-0.09108	0.01385
C	2.04609	0.61518	-1.72447
C	3.09297	1.38258	1.05349
C	4.03710	-1.17380	-0.27228
H	-3.13447	1.28211	-0.75058
H	-2.90882	-0.33865	-1.44254
C	-0.66737	1.50741	0.31326
H	-0.81098	-1.86794	1.07696
H	1.52476	-2.12382	1.01477
H	1.99023	-0.16551	-2.50135
H	2.85266	1.27863	-2.05290
H	1.13517	1.22851	-1.76181
H	2.32671	2.14875	1.19753
H	3.96394	1.85909	0.58849
H	3.39354	1.02802	2.04487
H	3.81101	-2.00553	-0.94697
H	4.38586	-1.59911	0.67476
H	4.86231	-0.59631	-0.70181
H	-6.82103	-0.55977	0.15012
H	-1.23287	2.03229	1.09516
H	-0.87165	2.02326	-0.63436
H	0.39343	1.63201	0.53688
Li	0.28957	-0.82455	-1.23001

Electronic Energy = -763.2363144
Zero-point corrected electronic energy=-

6bCA-C[1]Li

C	-5.46673	-0.35985	0.22336
C	-4.32366	-0.24126	-0.14213
C	-2.94170	-0.10065	-0.61747
O	-2.06087	-0.03955	0.47578
C	-0.71254	0.22015	0.09167
C	0.16250	-0.75867	0.62253
C	1.51818	-1.04172	0.46287
C	3.95015	-0.96992	0.00831
C	2.46997	0.39184	-1.42740
C	2.86686	1.04311	0.98684
H	-2.86916	0.80676	-1.23665
H	-2.69225	-0.95825	-1.26412
C	-0.48830	1.71978	0.07045
H	-0.40360	-1.58892	1.05169
H	1.84185	-1.96989	0.92643
H	3.85678	-1.82885	-0.66602
H	4.15902	-1.35166	1.01286
H	4.80748	-0.36828	-0.31335
H	2.52397	-0.43929	-2.14979
H	3.26795	1.08729	-1.70685
H	1.53361	0.94825	-1.57483
H	3.09745	0.65258	1.98264
H	1.97157	1.66038	1.07858
H	3.70010	1.68124	0.66532
H	-6.47361	-0.46225	0.56086
H	-0.60812	2.14161	1.07908
H	-1.23056	2.20714	-0.57129
H	0.49355	2.01871	-0.29673
C	2.66216	-0.13387	0.01425
Li	0.44316	-0.84463	-1.38124

Electronic Energy = -511.8232618
Zero-point corrected electronic energy=-

762.993512 Zero-point corrected Gibbs free energy=-763.039246	511.569235 Zero-point corrected Gibbs free energy=-511.611017
6bA-C^2Li	6bCA-C^2Li
C 3.35379 -2.44751 -0.20049 C 3.20873 -1.17515 -0.06494 C 2.69110 0.01418 0.28806 O 1.84704 0.68616 -0.60818 C -0.25506 1.64979 -1.02672 C -1.42579 1.00282 -1.08346 Si -2.01363 -0.38839 0.03495 C -0.56968 -1.57831 0.41140 C -2.68656 0.27022 1.66515 C -3.35170 -1.33451 -0.88477 H 3.10970 0.61425 1.09276 C 1.32966 2.76605 0.55497 H 0.00091 2.39256 -1.78537 H -2.09040 1.27461 -1.90649 H -0.15768 -1.29947 1.39155 H 0.17968 -1.45424 -0.38276 H -0.91532 -2.61653 0.44083 H -1.92016 0.83632 2.20501 H -3.02813 -0.54569 2.31099 H -3.53302 0.94133 1.49020 H -2.96772 -1.74696 -1.82310 H -4.19495 -0.67934 -1.12646 H -3.73412 -2.16369 -0.28087 H 4.13229 -2.94297 -0.76985 H 1.76516 3.34745 -0.26324 H 2.09830 2.61484 1.31733 H 0.51208 3.34073 1.00114 Li 1.70770 -2.14104 0.85097 C 0.81142 1.43435 0.01707 H 0.39928 0.84648 0.85384	C 2.90010 -2.48019 -0.25900 C 2.73124 -1.32630 0.28401 C 2.91087 -0.00185 0.48384 O 2.21043 0.94298 -0.26911 C -0.05231 0.45819 0.39777 C -1.30593 0.64062 -0.01821 C -2.91337 -0.54135 -1.47348 C -1.95494 -1.74996 0.49699 C -3.56838 0.13346 0.84698 H 3.44052 0.39263 1.35008 C 0.71176 2.77404 -0.35936 H 0.25692 -0.51025 0.78696 H -1.60477 1.61770 -0.40509 H -2.11496 -0.91815 -2.12052 H -3.75488 -1.24210 -1.51697 H -3.25304 0.41981 -1.87527 H -1.13385 -2.15062 -0.10712 H -2.78474 -2.46372 0.45975 H -1.61413 -1.68261 1.53551 H -3.91874 1.10911 0.49212 H -3.24705 0.24487 1.88756 H -4.41601 -0.56070 0.81860 H 2.34273 -3.38767 -0.06049 H 0.43658 2.55543 -1.39518 H 1.58582 3.42899 -0.36054 H -0.11708 3.29674 0.12512 C -2.41561 -0.38850 -0.02646 C 1.04586 1.49005 0.37540 H 1.32719 1.72730 1.41505 Li 4.11677 -1.15663 -1.12255
Electronic Energy = -763.2485226 Zero-point corrected electronic energy=-763.004752 Zero-point corrected Gibbs free energy=-763.049289	Electronic Energy = -511.8527544 Zero-point corrected electronic energy=-511.599836 Zero-point corrected Gibbs free energy=-511.642563
Anionic Intermediates	
6bA-C^1_anion	6bCA-C^1_anion
C -5.72154 -0.30671 -0.31582 C -4.51755 -0.25808 -0.40289 C -3.05126 -0.20712 -0.53369 O -2.45945 0.08806 0.70824 C -1.05158 0.24644 0.59259 C -0.25920 -0.82226 0.90021 C 1.14960 -1.02092 0.85308	C -5.45174 -0.39641 0.09913 C -4.28475 -0.29401 -0.19824 C -2.86762 -0.17683 -0.59533 O -2.05939 0.03955 0.52727 C -0.68742 0.26525 0.14790 C 0.16383 -0.78451 0.48951 C 1.53361 -1.04774 0.49571

Si	2.43992	-0.16429	-0.07147
C	1.91306	0.43088	-1.80935
C	3.30612	1.37293	0.69047
C	3.89983	-1.36950	-0.33272
H	-2.79171	0.55538	-1.28494
H	-2.68834	-1.17390	-0.91302
C	-0.63187	1.64534	0.28669
H	-0.85025	-1.67699	1.25189
H	1.48774	-1.94024	1.33465
H	1.26874	1.31531	-1.76141
H	1.35768	-0.36077	-2.32418
H	2.79448	0.68986	-2.41073
H	2.60283	2.19259	0.87549
H	4.10179	1.75075	0.03301
H	3.75558	1.10316	1.65374
H	3.59498	-2.21238	-0.96253
H	4.23518	-1.77496	0.62962
H	4.75558	-0.87265	-0.80673
H	-6.78247	-0.34731	-0.22052
H	-1.24307	2.35481	0.86441
H	-0.71107	1.94374	-0.77380
H	0.41535	1.78313	0.57822

Electronic Energy = -755.7142273
Zero-point corrected electronic energy=-755.476442
Zero-point corrected Gibbs free energy=-755.521877

C	2.38505	0.20911	-1.50931
C	2.90101	1.07728	0.81309
C	3.96003	-0.99898	-0.01272
H	-2.77402	0.65104	-1.31743
H	-2.56470	-1.09449	-1.12288
C	-0.42297	1.73993	0.07773
H	-0.42638	-1.64320	0.82671
H	1.81920	-2.05502	0.79247
H	1.36442	0.58252	-1.63181
H	2.47541	-0.67779	-2.14796
H	3.09220	0.97213	-1.86942
H	1.99396	1.67498	0.91508
H	3.69072	1.71178	0.37936
H	3.20862	0.77760	1.82112
H	3.86242	-1.90506	-0.62272
H	4.19322	-1.30479	1.01487
H	4.80375	-0.40982	-0.39822
H	-6.47516	-0.48533	0.38316
H	-1.24934	2.25243	-0.43597
H	0.48796	1.98771	-0.47327
H	-0.33672	2.21779	1.07691
C	2.65589	-0.18791	-0.04217

Electronic Energy = -504.2956255
Zero-point corrected electronic energy=-504.046874
Zero-point corrected Gibbs free energy=-504.088354

6bA-C^2_anion

C	-1.73339	2.54509	0.85289
C	-2.11155	1.72783	-0.07358
C	-2.51473	0.73316	-0.87397
O	-1.73590	-0.45202	-1.03760
C	-0.22084	-2.00237	-0.10027
C	1.07541	-1.66859	-0.17006
Si	1.79148	0.07067	0.00396
C	1.20680	1.17457	-1.39795
C	1.43386	0.87061	1.67218
C	3.67309	-0.15577	-0.13767
H	-3.42923	0.71437	-1.45473
C	-2.50597	-1.68633	0.91048
H	-0.53435	-3.03230	-0.29741
H	1.77630	-2.46930	-0.42508
H	0.11218	1.22413	-1.41011
H	1.54634	0.78348	-2.36360
H	1.59794	2.19116	-1.27309
H	0.42033	1.28879	1.71068
H	2.14153	1.69278	1.83640
H	1.55122	0.15242	2.49105
H	3.94371	-0.63405	-1.08601

6bCA-C^2_anion

C	-4.59515	0.80627	-0.98398
C	-3.98969	-0.14187	-0.33871
C	-3.29463	-0.95606	0.45926
O	-1.86897	-1.04156	0.46784
C	0.22356	-0.29401	-0.20815
C	1.31357	0.39579	0.13197
C	2.88712	-1.35438	-0.80634
C	3.41934	1.08160	-0.98206
C	3.48034	-0.05564	1.24487
H	-3.71465	-1.64400	1.18268
C	-1.39902	1.29564	0.96531
H	0.31685	-1.25953	-0.70507
H	1.19350	1.35397	0.64237
H	2.39664	-1.34459	-1.78531
H	2.43274	-2.15043	-0.20751
H	3.94557	-1.59813	-0.95656
H	2.93341	1.13664	-1.96167
H	4.48429	0.86290	-1.13184
H	3.33684	2.06703	-0.50960
H	3.03602	-0.82439	1.88523
H	3.40213	0.90469	1.76712

H	4.05803	-0.77933	0.67756
H	4.18451	0.81232	-0.09152
H	-1.05840	3.36089	0.55999
H	-2.90855	-2.50084	0.29612
H	-3.28779	-0.93889	1.07079
H	-2.19516	-2.09143	1.88014
C	-1.33109	-1.02522	0.19788
H	-0.94171	-0.22522	0.84457

Electronic Energy = -755.7122597
Zero-point corrected electronic energy=-755.473631
Zero-point corrected Gibbs free energy=-755.517039

H	4.54497	-0.28437	1.10854
H	-4.92518	0.56002	-2.00359
H	-0.95942	1.06716	1.94341
H	-2.46996	1.48008	1.07601
H	-0.93500	2.20293	0.56285
C	-1.20754	0.11947	0.01405
H	-1.63271	0.41049	-0.96369
C	2.75640	0.00185	-0.11055

Electronic Energy = -504.3150212
Zero-point corrected electronic energy=-504.064757
Zero-point corrected Gibbs free energy=-504.106213