Electronic Supplementary Information

Simultaneous CO_2 capture and functionalization: solvated electron precursors as novel catalysts

Benjamin A. Jackson and Evangelos Miliordos*

Department of Chemistry and Biochemistry, Auburn University, Auburn, AL 36849-5312, USA

Corresponding Author

* E-mail: emiliord@auburn.edu

Reactants, intermediates, and transition states for the gas-phase reaction pathways of $Li(X)_4 + CO_2 + 2\ H_2 \rightarrow Li(X)_4 + CH_2(OH)_2$ (X= NH_3, NH_2CH_3, $NH_2CH_2CH_3$, H_2O, CH_3OH) and $Li(Y)_4 + 2\ C_2H_4 \rightarrow Li(Y)_4 + C_5H_8O_2$ (Y= NH_3, NH_2CH_3) were optimized under density functional theory using the CAM-B3LYP functional and the cc-pVTZ (C, N, O) and aug-cc-pVTZ (H) basis sets. The task of locating transition states for the formic acid/methyldiol system proved to be one of significant challenge; for select structures alternative methods were employed to aid in their identification. For the eTS1 structure of $Li(NH_2CH_2CH_3)_4$ no transition state could be located- this is likely a result of the electron transfer from the SEP to CO_2 being barrierless due to the trend of decreasing I.E. for more larger ligands. The structure and energy reported was obtained using the eTS1 structure of $Li(NH_2CH_3)_4$, adding the additional methane to each ligand, and fixing the atoms of Li and CO_2 when optimizing. This same process was also used to obtain the eTS2 structure $Li(H_2O)_4$ starting from eTS2 of $Li(CH_3OH)_4$. For the OHTS2 and eTS1 structures of $Li(CH_3OH)_4$, these were located at the double-ζ (DZ) basis set level but could not be located at triple-ζ (TZ). As such, the energies reported are from single point TZ calculations using the optimized DZ geometry. For all ligands, the transition state CHTS2 could not be located at CAM-B3LYP (DZ or TZ). Instead, CHTS2 was located and optimized at the MP2 double-ζ level and energies reported are from single point CAM-B3LYP(TZ) calculations at the MP2 geometry. The CAM-B3LYP methodology was benchmarked using the higher level CCSD(T). To ensure these calculations were tractable, the cc-pVDZ (C, N, O) and aug-cc-pVDZ (H) basis sets were used and a correction to triple-ζ was approximated as $E^{CCSD(T)}(TZ) \approx E^{CCSD(T)}(DZ) + \{E^{MP2}(TZ) - E^{MP2}(DZ)\}$, where $E^{CCSD(T)}(DZ)$ is the single point energy at CCSD(T) double-ζ basis set while $E^{MP2}(TZ)$and $E^{MP2}(DZ)$ are the single point energies at MP2 under triple-ζ and double-ζ, respectively.

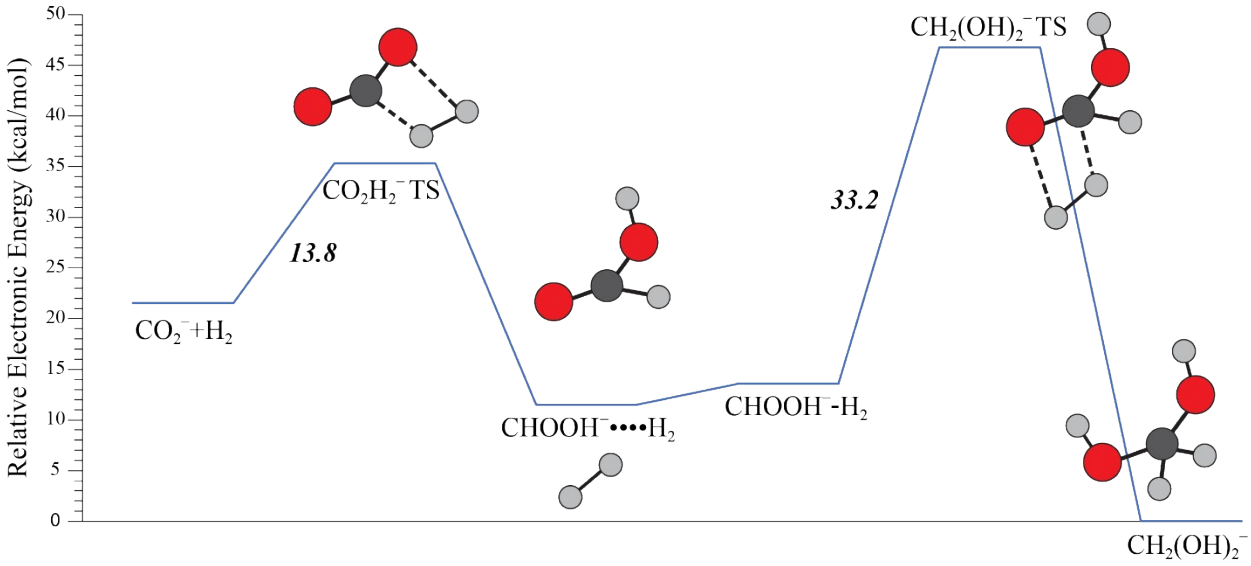

Figure S1. Reaction pathway of CO_2^- + $2H_2$→ $CH_2(OH)_2^-$. Structures of transition states and select intermediates are shown. Structures optimized at CAM-B3LYP with basis sets cc-pVTZ (C, O), aug-cc-pVTZ (H).

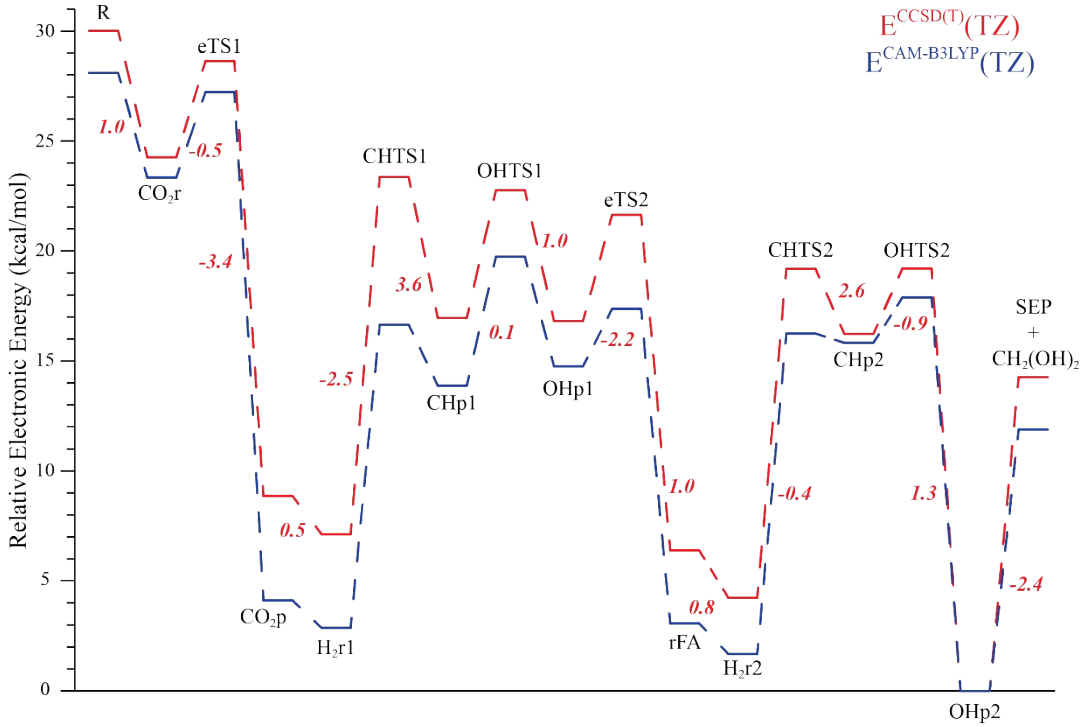

Figure S2. Comparison of CCSD(T) and CAM-B3LYP energetics of the $Li(H_2O)_4$ + CO_2 + $2H_2$ → $Li(H_2O)_4$ + $CH_2(OH)_2$. In red is the relative energy difference between the two methods calculated as ΔE(CAM-B3LYP)-Δ{$E^{CCSD(T)}$(TZ)}. See above for details.

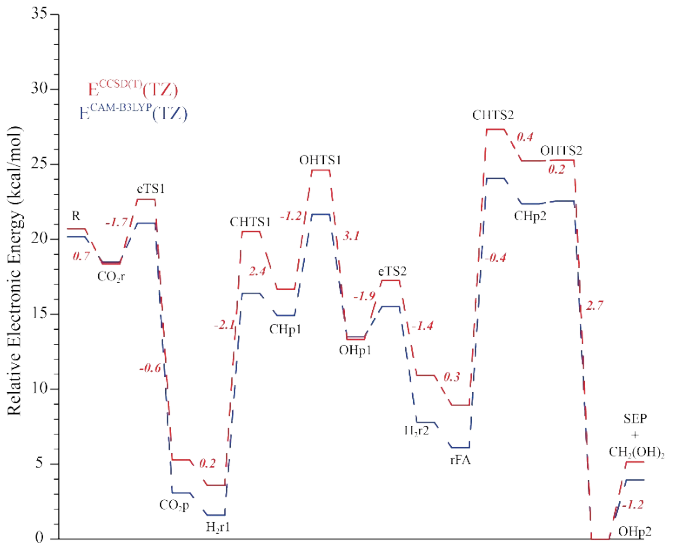

Figure S3. Comparison of CCSD(T) and CAM-B3LYP energetics of the $Li(NH_3)_4 + CO_2 + 2H_2 \rightarrow Li(NH_3)_4 + CH_2(OH)_2$. In red is the relative energy difference between the two methods calculated as $\Delta E(\text{CAM-B3LYP}) - \Delta\{E^{CCSD(T)}(TZ)\}$. See above for details.

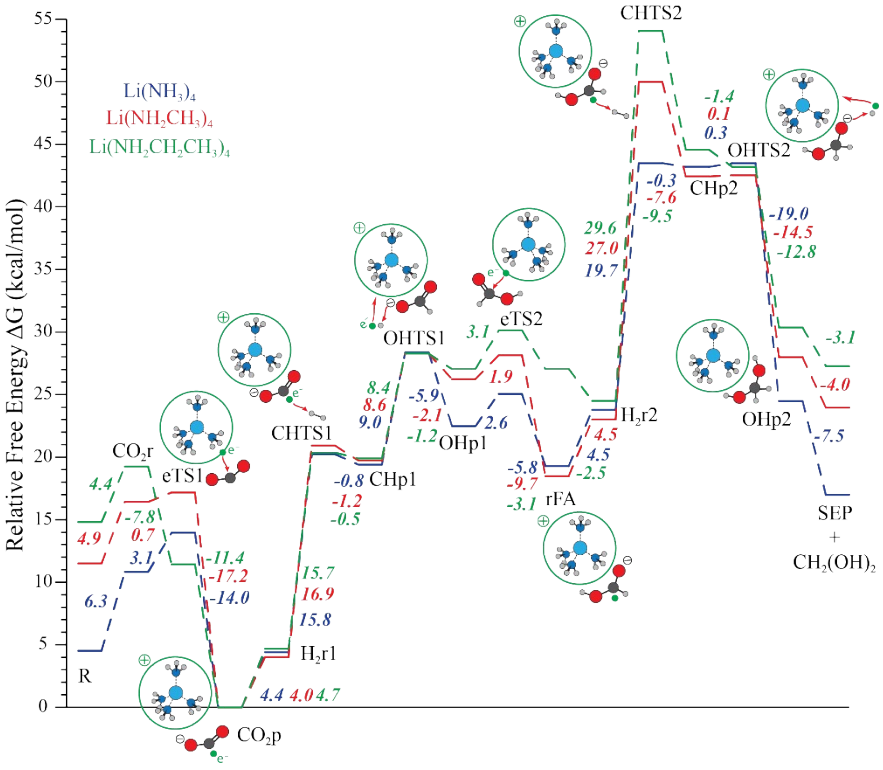

Figure S4. Relative Gibbs free energy at 298K of the reaction pathway for $Li(X)_4 + CO_2 + 2\ H_2 \rightarrow Li(X)_4 + CH_2(OH)_2$ (X= NH_3, NH_2CH_3, $NH_2CH_2CH_3$). Graphical representations of transition states and select intermediates are given as figure insets. A green dot is used to indicate the movement of the SEP e^- throughout the pathway. Activation barriers are given in kcal/mol. Relative electronic energies are zeroed to the lowest point of the pathway.

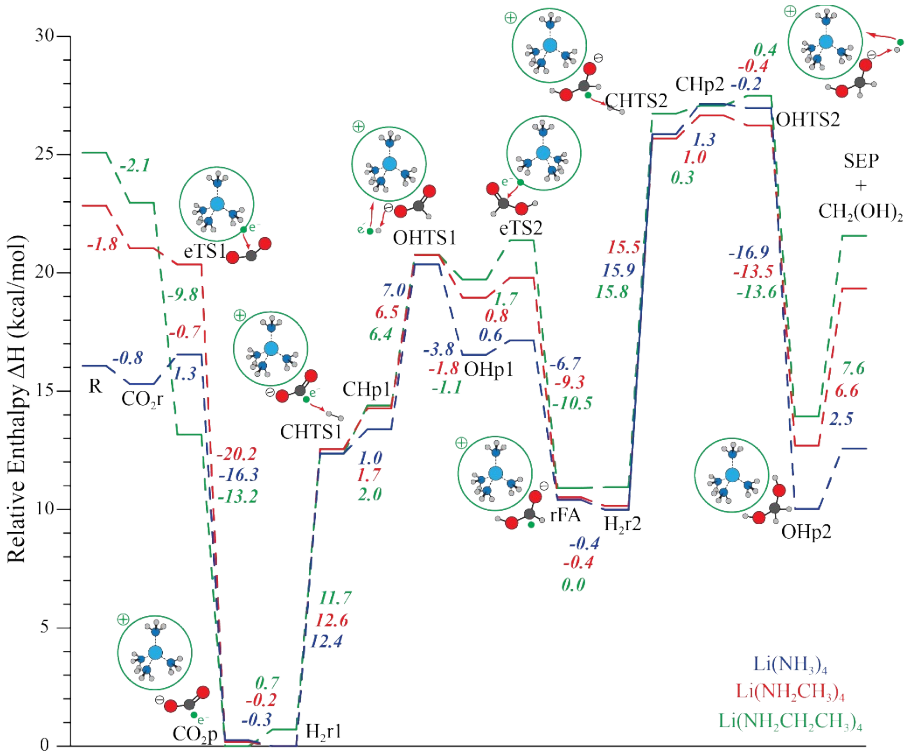

Figure S5. Relative enthalpy at 298K of the reaction pathway for $Li(X)_4 + CO_2 + 2\ H_2 \rightarrow Li(X)_4 + CH_2(OH)_2$ (X= NH_3, NH_2CH_3, $NH_2CH_2CH_3$). Graphical representations of transition states and select intermediates are given as figure insets. A green dot is used to indicate the movement of the SEP e^- throughout the pathway. Activation barriers are given in kcal/mol. Relative electronic energies are zeroed to the lowest point of the pathway.

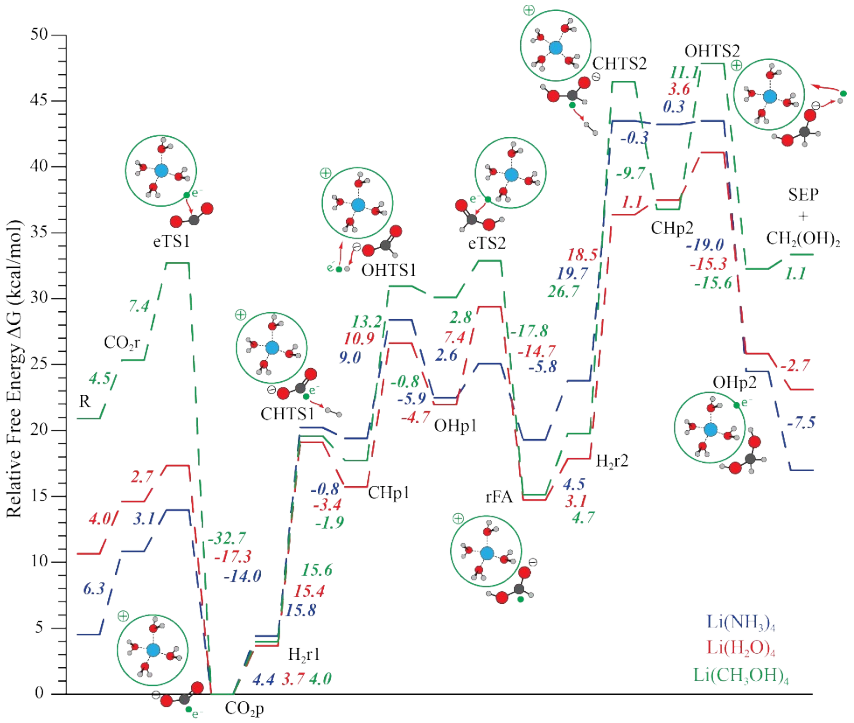

Figure S6. Relative Gibbs free energy at 298K of the reaction pathway for $Li(X)_4 + CO_2 + 2\ H_2 \rightarrow Li(X)_4 + CH_2(OH)_2$ (X= NH_3, H_2O, CH_3OH). Graphical representations of transition states and select intermediates are given as figure insets. A green dot is used to indicate the movement of the SEP e^- throughout the pathway. Activation barriers are given in kcal/mol. Relative electronic energies are zeroed to the lowest point of the pathway.

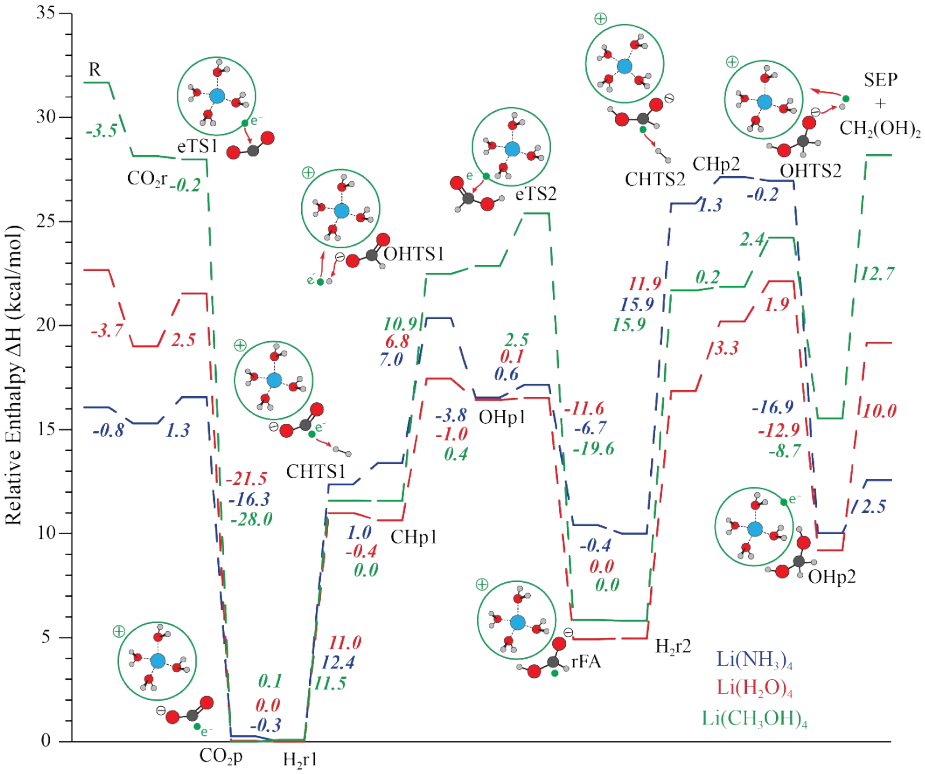

Figure S7. Relative enthalpy at 298K of the reaction pathway for $Li(X)_4 + CO_2 + 2\ H_2 \rightarrow Li(X)_4 + CH_2(OH)_2$ (X= NH_3, H_2O, CH_3OH). Graphical representations of transition states and select intermediates are given as figure insets. A green dot is used to indicate the movement of the SEP e^- throughout the pathway. Activation barriers are given in kcal/mol. Relative electronic energies are zeroed to the lowest point of the pathway.

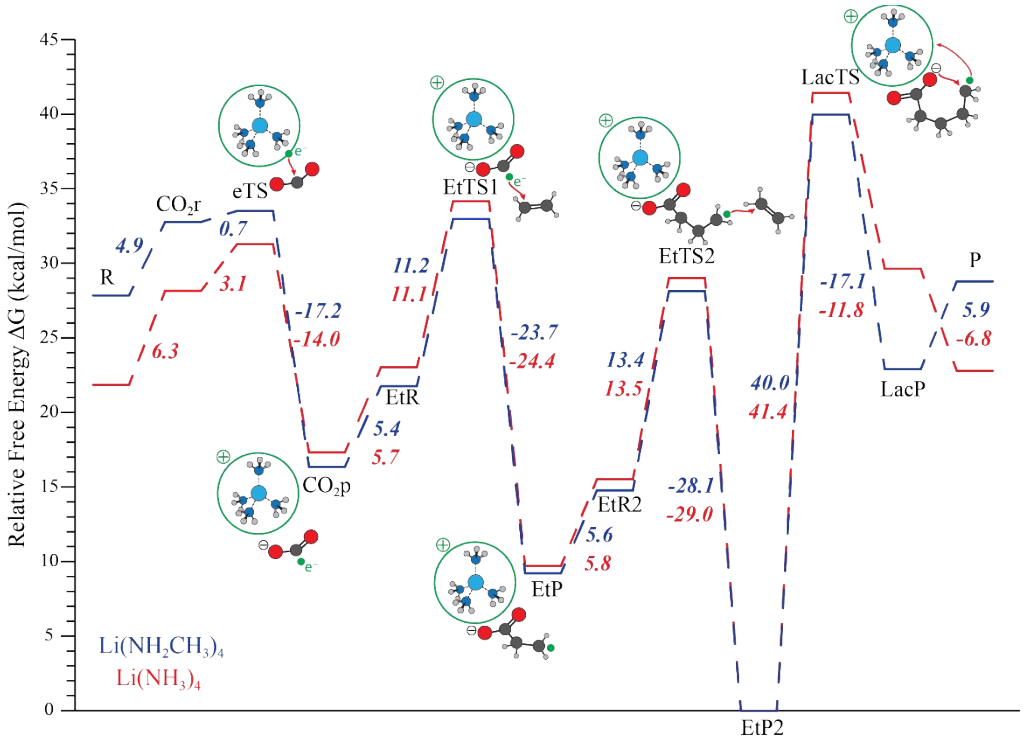

Figure S8. Relative Gibbs free energy at 298K of the reaction pathway for $Li(X)_4 + 2\ C_2H_4 \rightarrow Li(X)_4 + C_5H_8O_2$ (X= NH_3, NH_2CH_3). Graphical representations of transition states and select intermediates are given as figure insets. A green dot is used to indicate the movement of the SEP e^- throughout the pathway. Activation barriers are given in kcal/mol. Relative electronic energies are zeroed to the lowest point of the pathway.

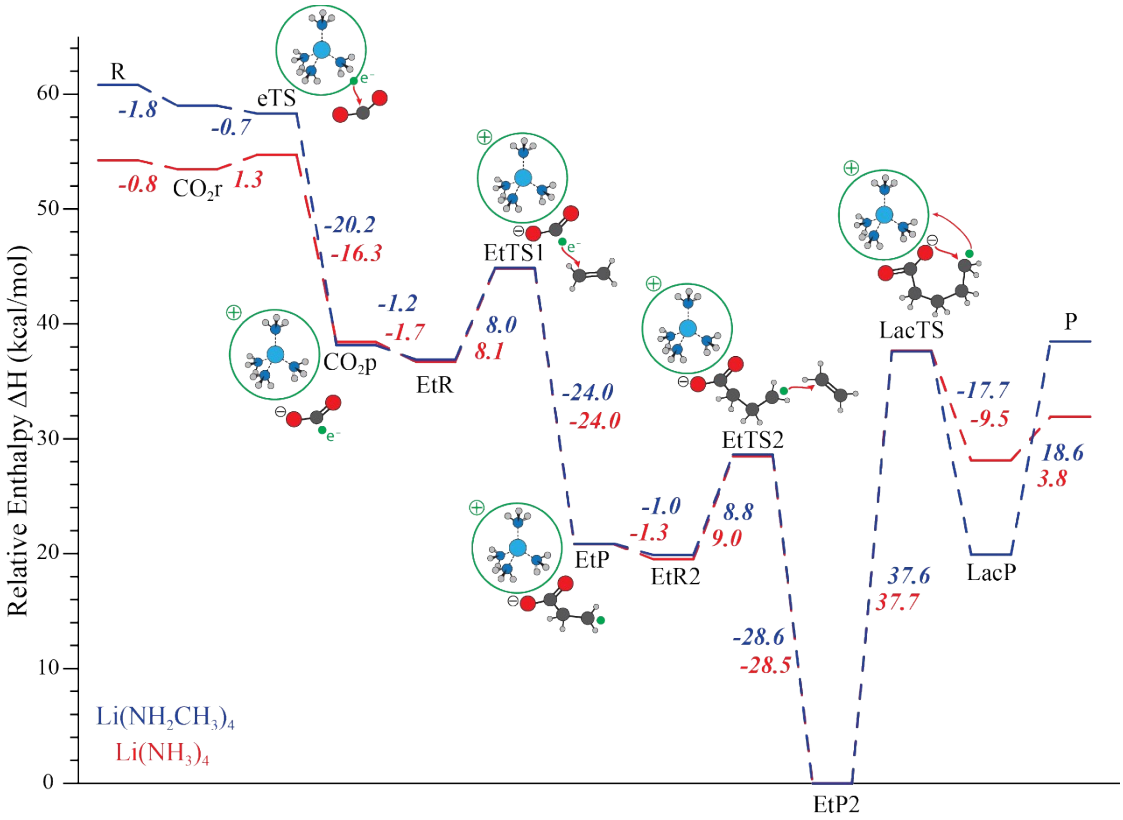

Figure S9. Relative enthalpy at 298K of the reaction pathway for $Li(X)_4 + 2\ C_2H_4 \rightarrow Li(X)_4 + C_5H_8O_2$ (X= NH_3, NH_2CH_3). Graphical representations of transition states and select intermediates are given as figure insets. A green dot is used to indicate the movement of the SEP e^- throughout the pathway. Activation barriers are given in kcal/mol. Relative electronic energies are zeroed to the lowest point of the pathway.

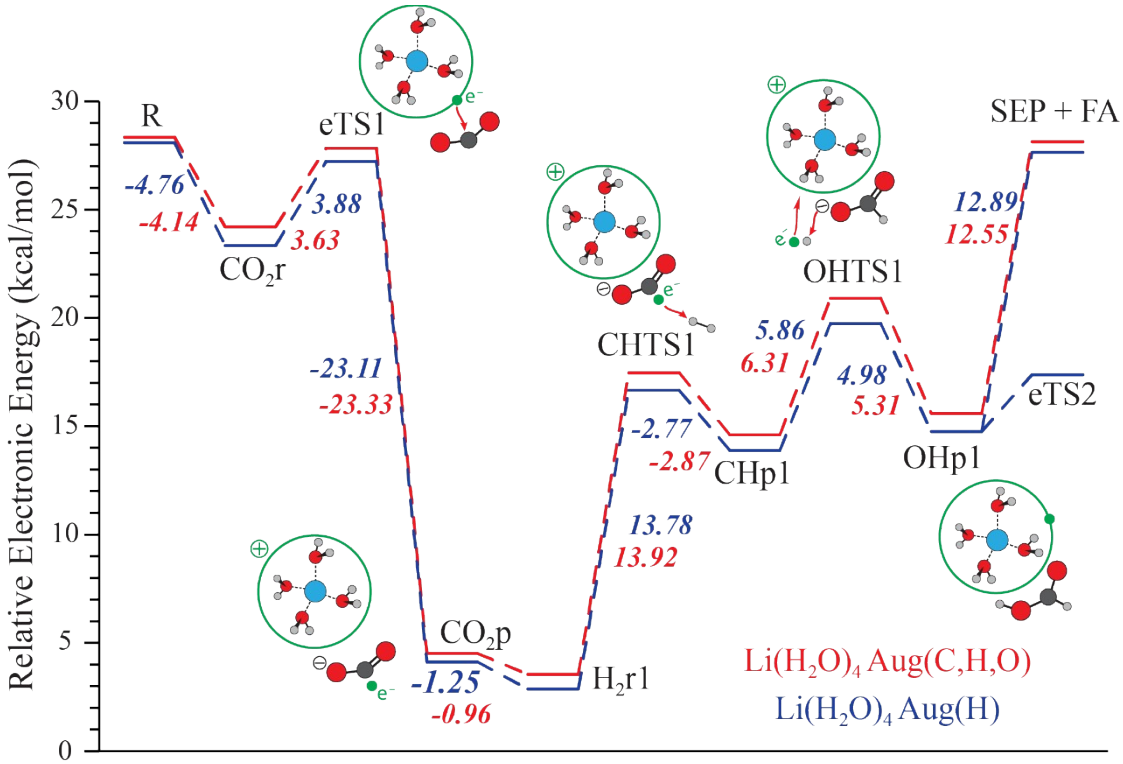

Figure S10. Effect of augmented functions on the reaction pathway for $Li(H_2O)_4 + CO_2 + H_2 \rightarrow Li(H_2O)_4 + CO_2H_2$. The pathway in red are the structures optimized with aug-cc-pVTZ (C, O, H), cc-pVTZ (Li) and in blue is those optimized with aug-cc-pVTZ (H), cc-pVTZ (Li, C, O). Graphical representations of transition states and select intermediates are given as figure insets. A green dot is used to indicate the movement of the SEP e^- throughout the pathway. Activation barriers are given in kcal/mol. Relative electronic energies are zeroed to the lowest point of the pathway (not shown). These results indicate the effect of augmented functions for C and O to be minimal.

Table S1. Cartesian Coordinates (Å) for the reactants, products, and intermediates of the $Li(NH_3)_4 + CO_2 + 2H_2 \rightarrow Li(NH_3)_4 + CH_2(OH)_2$ reaction pathway.

$Li(NH_3)_4$

Li	0.000009	-0.000012	-0.000099
N	-0.002118	-2.055733	0.121696
N	1.790986	0.638982	-0.790750
N	-1.545383	0.617417	-1.213109
N	-0.243470	0.799328	1.882126
H	0.115071	-2.493213	-0.788954
H	-0.871010	-2.415284	0.509192
H	0.748278	-2.405079	0.712681
H	1.834706	1.651999	-0.870016
H	1.953092	0.265471	-1.722743
H	2.583914	0.355820	-0.220235
H	-0.249736	1.816274	1.868390
H	0.501427	0.520031	2.515792
H	-1.117792	0.507308	2.311889
H	-1.581365	1.629988	-1.301480
H	-2.451702	0.322489	-0.858137
H	-1.465022	0.244279	-2.155821

CO_2

C	0.000000	0.000000	-0.000010
O	0.000000	0.000000	-1.155618
O	-0.000000	-0.000000	1.155626

H_2

H	0.000000	0.000000	0.372728
H	0.000000	0.000000	-0.372728

Formic Acid

C	0.133141	0.359641	0.000048
O	-1.051295	-0.277483	-0.000051
O	1.167788	-0.219220	0.000006
H	0.043055	1.457378	-0.000214
H	-1.773852	0.358403	0.000292

Methyldiol

C	0.000000	0.000000	0.528321
O	0.000000	1.165769	-0.246760
H	-0.889425	-0.070276	1.155262
H	0.889425	0.070276	1.155262
O	-0.000000	-1.165769	-0.246760
H	-0.808755	1.191516	-0.766144
H	0.808755	-1.191516	-0.766144

CO_2r

Li	1.333803	-0.001072	-0.011985
N	3.288410	-0.001790	-0.674313
N	1.437284	0.005041	2.045205
N	0.482066	1.749026	-0.700506
N	0.480236	-1.753232	-0.692624
H	3.794477	0.814733	-0.336390
H	3.384422	-0.003755	-1.687587
H	3.796385	-0.815695	-0.333014
H	0.551863	0.006969	2.544983
H	1.954490	0.821459	2.364792
H	1.954513	-0.808861	2.371057
H	-0.473211	-1.960927	-0.410612
H	1.060038	-2.514123	-0.346333
H	0.506496	-1.809757	-1.707407
H	-0.469668	1.962219	-0.416791
H	0.505285	1.799153	-1.715720
H	1.065788	2.509953	-0.360850
C	-2.796321	0.000405	0.011418
O	-2.791412	-1.156081	0.010163
O	-2.792379	1.156845	0.009460

eTS1

Li	1.293410	0.027261	-0.000221
N	3.364924	0.057270	0.000105
N	0.564372	1.955620	-0.000046
N	0.579950	-0.990143	-1.651582
N	0.580585	-0.990700	1.651083
H	3.735682	0.535128	-0.815264
H	3.760648	-0.877679	-0.000233
H	3.735234	0.534370	0.816127
H	-0.454999	1.930284	0.000547
H	0.838609	2.497130	-0.815237
H	0.839599	2.497302	0.814699
H	-0.345116	-1.335355	1.401755
H	0.460091	-0.408329	2.475111
H	1.125227	-1.798050	1.940656
H	-0.345463	-1.335404	-1.401911
H	1.124772	-1.797069	-1.942017
H	0.458722	-0.407278	-2.475156
C	-2.596192	-0.028498	0.000152
O	-2.564809	1.141235	0.000533
O	-2.293302	-1.162507	-0.000065

CO_2p

Li	1.240280	0.024100	-0.012381
N	3.327989	-0.051503	0.129458
N	0.524386	1.895792	-0.446936
N	0.482236	-1.267950	-1.436119
N	0.296483	-0.532660	1.737640
H	3.774493	0.282797	-0.715506
H	3.662654	-0.992932	0.293162
H	3.663174	0.522382	0.893309
H	-0.478068	1.688418	-0.308671
H	0.621815	2.252097	-1.389903
H	0.749636	2.665629	0.171388
H	0.042075	0.242095	2.338621
H	0.606590	-1.282158	2.343150
H	-0.575619	-0.841504	1.288861
H	-0.468493	-1.307819	-1.044210
H	0.810002	-2.223023	-1.510355
H	0.396902	-0.918855	-2.382807
C	-2.577155	-0.045518	-0.027190
O	-2.184932	1.116914	-0.004583
O	-2.000159	-1.140923	0.046451

H_2r1

Li	1.358767	-0.083329	-0.013311
N	3.408324	-0.474941	0.151003
N	0.942490	1.861841	-0.515856
N	0.413762	-1.288040	-1.401300
N	0.331733	-0.423687	1.745713
H	3.595028	-1.451424	0.342800
H	3.823061	0.061901	0.902693
H	3.905817	-0.236018	-0.697864
H	-0.077010	1.817697	-0.361263
H	1.081265	2.161986	-1.473054
H	1.293418	2.609984	0.069617
H	0.181963	0.411631	2.299022
H	0.533712	-1.172873	2.395681
H	-0.572338	-0.633701	1.305750
H	-0.534442	-1.173231	-1.020025
H	0.594763	-2.283401	-1.442724
H	0.388055	-0.960861	-2.359279
C	-2.429532	0.431450	-0.022802
O	-1.849594	1.511489	-0.005517
O	-2.042212	-0.745031	0.053964
H	-4.372511	-2.956151	-0.021501
H	-3.879602	-2.392128	-0.007587

CHTS1

Li	1.387449	0.019223	-0.002808
N	3.479043	-0.064508	0.021038
N	0.653881	1.929482	-0.088406
N	0.545754	-1.000924	-1.588528
N	0.513506	-0.852097	1.652148
H	3.877256	0.387698	-0.792651
H	3.821396	-1.017282	0.031591
H	3.858514	0.398993	0.837332
H	-0.354034	1.699445	-0.059626
H	0.804900	2.473792	-0.928977
H	0.832321	2.555129	0.687732
H	0.349902	-0.243201	2.444487
H	0.810615	-1.743328	2.028973
H	-0.398737	-1.002505	1.199910
H	-0.380454	-1.098425	-1.150219
H	0.845451	-1.929230	-1.858957

CHp1

Li	1.372000	0.055054	0.000125
N	3.465557	0.068014	-0.000944
N	0.542463	1.925111	0.003254
N	0.551317	-0.921647	-1.620375
N	0.552792	-0.926843	1.618180
H	3.853450	-0.867092	-0.007363
H	3.830991	0.539182	0.817263
H	3.830071	0.549981	-0.813248
H	-0.447947	1.623375	0.002236
H	0.666791	2.522619	-0.804856
H	0.666144	2.519292	0.813914
H	0.364882	-0.361931	2.437132
H	0.887086	-1.821148	1.954174
H	-0.353382	-1.094140	1.155519
H	-0.354360	-1.090439	-1.157308
H	0.884995	-1.814752	-1.960138

OHTS1

Li	1.376701	0.056532	-0.000036
N	3.464541	0.214274	0.000119
N	0.434575	1.885706	-0.000459
N	0.677179	-1.010694	-1.626184
N	0.677012	-1.010029	1.626474
H	3.878789	-0.709876	-0.004806
H	3.819869	0.694913	0.817491
H	3.819699	0.703515	-0.812207
H	-0.570061	1.655811	-0.000251
H	0.591773	2.474876	-0.809637
H	0.592017	2.475328	0.808342
H	0.658072	-0.578680	2.542591
H	0.970200	-1.969910	1.765983
H	-0.289355	-1.055128	1.295942
H	-0.289285	-1.055345	-1.295864
H	0.970093	-1.970737	-1.765157

H	0.412818	-0.479675	-2.446343
C	-2.486480	-0.018973	-0.000702
O	-2.078759	1.144313	-0.001547
O	-1.861456	-1.097836	0.012244
H	-3.685305	-0.140675	-0.013562
H	-4.861681	-0.260056	-0.026397

OHp1

Li	-1.361508	0.107075	0.003873
N	-3.423676	0.422910	-0.038443
N	-0.897674	-1.120262	1.599711
N	-0.920990	-0.952498	-1.717728
N	-0.293490	1.875714	0.177501
H	-3.837760	0.896888	0.756779
H	-3.834026	-0.504908	-0.076379
H	-3.731762	0.911286	-0.872388
H	0.107816	-1.022602	1.708295
H	-1.052675	-2.084950	1.317110
H	-1.317050	-1.010847	2.516666
H	-0.529519	2.411242	1.004952
H	-0.417417	2.497551	-0.613256
H	0.704307	1.673442	0.232660
H	-0.315145	-1.740102	-1.471278
H	-0.421941	-0.441794	-2.443828
H	-1.727446	-1.372277	-2.176073
C	2.767504	-0.092527	-0.241963
O	2.683073	1.081351	-0.019552
O	1.945562	-0.975987	0.317366
H	3.517516	-0.526799	-0.912338
H	2.056332	-1.876166	-0.060564

H_2r2

Li	1.421853	-0.000387	-0.012932
N	0.527369	-1.369530	-1.272640
N	0.444868	-0.158646	1.791269
N	3.492868	-0.265338	0.202621
N	0.901005	1.843129	-0.780499
C	-2.217093	-0.115303	-0.459455
O	-2.257336	-1.304628	0.345051
O	-1.550246	0.844532	0.070017
H	-3.203692	0.092190	-0.902098
H	-2.889933	-1.906743	-0.054680
H	0.652323	0.403702	2.606695
H	0.183245	-1.076945	2.128695
H	-0.408890	0.226184	1.348461
H	0.999650	2.037085	-1.768765
H	1.108865	2.706383	-0.294704
H	-0.095756	1.623135	-0.599773
H	3.675672	-0.532339	1.161798
H	3.983861	0.602447	0.028355
H	3.903661	-0.972052	-0.393921
H	0.411184	-2.294421	-0.876591
H	0.840548	-1.494622	-2.227135
H	-0.419868	-0.968880	-1.312038
H	-3.132051	2.534626	0.476645
H	-3.673930	3.046690	0.568778

OHTS2

Li	-1.422815	-0.062852	-0.030679
N	-0.429296	-1.519941	-1.116062
N	-1.011416	1.758438	-0.900054
N	-3.487207	-0.388249	0.158206
N	-0.494413	-0.056734	1.793961
C	2.626690	0.276083	-0.139351
O	2.271933	-1.128498	0.119899
O	1.525647	1.027358	-0.032506
H	3.080053	-1.643335	0.198866
H	-1.218823	2.597133	-0.370980
H	-1.199327	1.974976	-1.870531
H	0.004051	1.602775	-0.796586
H	-0.226044	-0.942355	2.205408

H	0.362554	-0.353584	-2.436952
C	-2.522709	-0.212267	0.000084
O	-2.128799	0.971375	0.000142
O	-1.808770	-1.243878	-0.000336
H	-3.617842	-0.371749	0.000390
H	-3.837525	2.296407	-0.000895

eTS2

Li	1.423305	-0.025903	0.051707
N	3.470249	-0.365443	0.244389
N	0.337200	-0.283796	1.791436
N	0.931137	1.868628	-0.626813
N	0.711210	-1.336230	-1.366060
C	-2.445652	0.211417	-0.386081
O	-2.872217	-0.892942	0.280332
O	-1.758917	1.041397	0.197933
H	-2.919198	0.384961	-1.350428
H	-3.332564	-1.478935	-0.334269
H	-0.528813	0.169940	1.491840
H	0.626456	0.151743	2.658175
H	0.100394	-1.243873	2.009832
H	0.708921	-2.323448	-1.116193
H	1.151409	-1.285851	-2.282900
H	-0.275195	-1.095343	-1.528526
H	-0.077560	1.823715	-0.471961
H	1.074905	1.998091	-1.620796
H	1.271323	2.704462	-0.167654
H	3.981159	0.198509	0.913598
H	3.906042	-0.227649	-0.660570
H	3.617218	-1.336867	0.494435

CHTS2

C	-2.409819	0.339623	-0.088321
H	-2.363613	0.429783	-1.258475
H	-2.159683	0.397659	-2.593606
Li	1.412675	-0.040823	-0.010137
N	0.396283	-1.379007	-1.277151
N	0.477627	-0.334209	1.837841
N	3.535065	-0.268163	0.043953
N	0.794376	1.823555	-0.720160
O	-2.159181	-1.113671	0.160177
O	-1.520683	1.081041	0.523630
H	-3.479765	0.520631	0.187786
H	-2.967749	-1.582973	-0.103530
H	0.736948	0.059756	2.745144
H	0.122276	-1.271780	2.045335
H	-0.374026	0.190578	1.522189
H	0.682532	1.988880	-1.723849
H	1.065317	2.732594	-0.336787
H	-0.177559	1.645597	-0.344001
H	3.864904	-0.798734	0.854174
H	3.982867	0.649054	0.116925
H	3.964736	-0.714833	-0.769895
H	0.654618	-2.362790	-1.385837
H	0.221247	-1.044444	-2.228743
H	-0.536697	-1.388429	-0.828326

OHp2

Li	1.555604	0.056738	-0.039659
N	0.475366	1.653648	0.705326
N	0.557529	-0.966896	-1.536596
N	3.420408	0.664343	-0.701246
N	1.943517	-1.250872	1.509826
C	-3.136008	-0.093532	0.162320
O	-2.558338	1.154246	-0.141010
O	-2.249310	-1.161311	-0.022701
H	-2.465705	1.232537	-1.095321
H	0.966413	-1.891390	-1.634521
H	0.594536	-0.534042	-2.454026
H	-0.423530	-1.100608	-1.301578
H	2.542004	-0.822944	2.215991

H	0.658607	-0.579784	-2.542515
C	-2.674528	-0.008271	0.000041
O	-2.390324	1.179509	0.000056
O	-1.808310	-0.967555	-0.000031
H	-3.723283	-0.333815	0.000094
H	-2.354147	-2.121570	-0.000001

rFA

Li	-1.361508	0.107075	0.003873
N	-3.423676	0.422910	-0.038443
N	-0.897674	-1.120262	1.599711
N	-0.920990	-0.952498	-1.717728
N	-0.293490	1.875714	0.177501
H	-3.837760	0.896888	0.756779
H	-3.834026	-0.504908	-0.076379
H	-3.731762	0.911286	-0.872388
H	0.107816	-1.022602	1.708295
H	-1.052675	-2.084950	1.317110
H	-1.317050	-1.010847	2.516666
H	-0.529519	2.411242	1.004952
H	-0.417417	2.497551	-0.613256
H	0.704307	1.673442	0.232660
H	-0.315145	-1.740102	-1.471278
H	-0.421941	-0.441794	-2.443828
H	-1.727446	-1.372277	-2.176073
C	2.767504	-0.092527	-0.241963
O	2.683073	1.081351	-0.019552
O	1.945562	-0.975987	0.317366
H	3.517516	-0.526799	-0.912338
H	2.056332	-1.876166	-0.060564

CHp2

Li	-1.417123	-0.063831	-0.033510
N	-0.455527	-1.687195	-0.884993
N	-0.943375	1.602234	-1.147999
N	-3.494356	-0.306048	0.176104
N	-0.513784	0.169723	1.790715
C	2.603572	0.285232	-0.153503
O	2.284412	-1.131021	0.128053
O	1.499065	1.013396	-0.017808
H	3.102241	-1.636406	0.137543
H	-1.197805	2.524447	-0.816060
H	-1.035852	1.623745	-2.155477
H	0.060938	1.473384	-0.919659
H	-0.269788	-0.655112	2.324910
H	-0.744561	0.891390	2.462014
H	0.352105	0.478714	1.314402
H	-3.948189	-0.998293	-0.405886
H	-3.931646	0.586174	-0.017626
H	-3.693266	-0.538883	1.140922
H	0.508779	-1.525610	-0.575809
H	-0.440356	-1.694919	-1.897429
H	-0.707665	-2.623221	-0.592792
H	3.014486	0.306555	-1.177845
H	3.400326	0.569042	0.553424
H	1.741662	2.189092	1.228171

H	-0.743309	0.556936	2.559584	H	2.430017	-2.090364	1.196439
H	0.360649	0.336655	1.378491	H	1.111767	-1.573381	2.005158
H	-3.967577	-0.703278	-0.675027	H	3.451162	1.301526	-1.491907
H	-3.901286	0.495374	0.428349	H	3.966320	-0.153707	-0.959626
H	-3.687183	-1.052351	0.895511	H	3.921115	1.114433	0.060727
H	0.515579	-1.430994	-0.730914	H	-0.528132	1.578253	0.551053
H	-0.358804	-1.310713	-2.104363	H	0.766139	2.559528	0.350835
H	-0.691814	-2.495039	-1.043969	H	0.619182	1.677918	1.710654
H	3.064311	0.307089	-1.148992	H	-3.989646	-0.290271	-0.484350
H	3.397413	0.552576	0.597468	H	-3.461369	-0.023925	1.198459
H	1.656107	1.941131	1.154330	H	-1.667597	-1.237626	0.745589

Table S2. Cartesian Coordinates (Å) for the reactants, products, and intermediates of the $Li(NH_2CH_3)_4 + CO_2 + 2H_2 \rightarrow Li(NH_2CH_3)_4 + CH_2(OH)_2$ reaction pathway.

$Li(NH_2CH_3)_4$			
Li	0.000082	-0.268028	0.000075
N	0.473285	0.826367	-1.696485
N	-1.534619	-1.571332	-0.470398
N	1.534997	-1.571240	0.470062
N	-0.473227	0.826124	1.696735
H	0.870764	0.096000	-2.281813
C	1.399822	1.961430	-1.613232
H	-0.380889	1.109458	-2.164231
H	-1.570252	-2.216047	0.318669
H	-1.163893	-2.128468	-1.240050
C	-2.897571	-1.130976	-0.799337
H	-0.869989	0.095624	2.282375
C	-1.400586	1.960522	1.613526
H	0.380919	1.109936	2.164089
H	1.164457	-2.128868	1.239442
C	2.897844	-1.130677	0.799162
H	1.570768	-2.215538	-0.319346
H	3.316193	-0.583836	-0.043693
H	3.572144	-1.955380	1.038050
H	2.867840	-0.457957	1.654559
H	-2.321342	1.638645	1.131797
H	-0.961957	2.743510	0.998181
H	-1.654855	2.389291	2.584846
H	2.320650	1.640307	-1.131135
H	0.960449	2.744255	-0.998209
H	1.654108	2.390156	-2.584567
H	-2.867710	-0.457764	-1.654352
H	-3.316131	-0.584732	0.043800
H	-3.571618	-1.955737	-1.038734

CO_2r			
Li	0.973686	0.322844	-0.144200
N	3.041809	0.168478	-0.300889
N	0.483721	2.275193	-0.612299
N	0.079025	-0.769937	-1.654755
N	0.150713	-0.204753	1.684549
H	3.175022	0.554453	-1.232176
C	3.698218	-1.140592	-0.206574
H	3.484952	0.825363	0.331726
H	-0.534400	2.276009	-0.683623
H	0.801598	2.398181	-1.573344
C	0.913869	3.427587	0.192608
H	0.174980	0.604235	2.294599
C	0.644198	-1.386807	2.398674
H	-0.825264	-0.331033	1.436746
H	-0.823572	-0.310454	-1.775108
C	-0.122598	-2.221481	-1.557709
H	0.590243	-0.548887	-2.507080
H	0.837572	-2.717392	-1.427273
H	-0.611642	-2.650362	-2.434475
H	-0.737069	-2.441830	-0.687306
H	1.680247	-1.228429	2.691919
H	0.616111	-2.247990	1.734138
H	0.068972	-1.628822	3.294633
H	3.243677	-1.820988	-0.923606
H	3.543983	-1.554168	0.787922
H	4.771580	-1.106968	-0.402958
H	2.001054	3.456114	0.238753
H	0.537648	3.323476	1.208783
H	0.564294	4.383285	-0.202861
C	-3.747846	-0.107119	0.058848
O	-4.671809	0.471276	-0.315985
O	-2.838561	-0.710615	0.457468

eTS1			
Li	-0.864777	0.029861	-0.317926
N	-2.870011	-0.361435	-0.734746
N	0.302801	-0.935460	-1.726170
N	-0.441325	2.024854	-0.636887
N	-0.296077	-0.520777	1.596329
H	-2.999557	0.128792	-1.613619
C	-3.880216	0.071031	0.236786
H	-2.987621	-1.345081	-0.947374
H	1.166730	-0.392928	-1.678725
H	-0.070049	-0.736981	-2.650672
C	0.624570	-2.364552	-1.619096
H	0.713167	-0.491648	1.487282
C	-0.704193	-1.822000	2.134398
H	-0.520906	0.212683	2.257897
H	0.575898	2.040711	-0.526198
C	-1.031474	3.119202	0.145915
H	-0.582405	2.204813	-1.629099
H	-2.109336	3.138806	-0.004551
H	-0.632215	4.100844	-0.116054
H	-0.843458	2.951338	1.204936
H	-0.439292	-2.604339	1.426316
H	-1.785151	-1.844308	2.262351
H	-0.242242	-2.062996	3.093932
H	-3.749318	1.130969	0.443353
H	-3.736313	-0.467094	1.171432
H	-4.907461	-0.089066	-0.096501
H	-0.291727	-2.952538	-1.641495
H	1.123592	-2.547954	-0.670291
H	1.278961	-2.720866	-2.416951
C	3.441710	0.346637	0.258747
O	4.323045	1.064883	0.041887
O	2.684822	-0.476749	0.604065

CO_2p			
Li	-0.692997	-0.038287	-0.419278
N	-2.678725	-0.377240	-0.999102
N	0.635473	-1.081770	-1.624801
N	-0.111465	1.946988	-0.619810
N	-0.473846	-0.539851	1.562422
H	-2.791027	-0.204123	-1.989827
C	-3.636399	0.422413	-0.229887
H	-2.854624	-1.364625	-0.861785
H	1.404227	-0.416706	-1.490327
H	0.424298	-1.078756	-2.614903
C	1.093786	-2.415869	-1.222607
H	0.548043	-0.429565	1.539090
C	-0.830291	-1.859701	2.083040
H	-0.813576	0.175555	2.192915
H	0.878394	1.729746	-0.777308
C	-0.219437	2.831767	0.543658
H	-0.435423	2.431049	-1.447615
H	-1.265684	2.993645	0.803419
H	0.249882	3.806408	0.393364
H	0.272038	2.359860	1.391902
H	-0.435853	-2.628252	1.421275
H	-1.914338	-1.974288	2.113427
H	-0.442071	-2.053890	3.085559
H	-3.430698	1.478592	-0.390268
H	-3.500540	0.218896	0.830082
H	-4.680282	0.231079	-0.487139
H	0.267574	-3.126416	-1.251799
H	1.467948	-2.362160	-0.202968
H	1.898867	-2.803588	-1.850694
C	2.931765	0.521257	0.344440
O	2.607660	0.914906	-0.784532

H_2r1			
Li	-0.826316	-0.022519	-0.405429
N	-2.853806	-0.419307	-0.759972
N	0.388529	-0.934741	-1.819565
N	-0.341806	1.993718	-0.550557
N	-0.341509	-0.627702	1.498531
H	-3.098818	-0.182536	-1.712908
C	-3.738445	0.274487	0.180742
H	-2.970952	-1.421505	-0.678224
H	1.147970	-0.252799	-1.725727
H	0.065265	-0.872598	-2.776959
C	0.927925	-2.275569	-1.568056
H	0.667449	-0.483078	1.366778
C	-0.600212	-1.987444	1.973200
H	-0.623199	0.036891	2.208367
H	0.634768	1.828075	-0.815470
C	-0.369002	2.816929	0.661757
H	-0.764697	2.502249	-1.316843
H	-1.390658	2.924224	1.026196
H	0.049178	3.815555	0.518419
H	0.216847	2.325417	1.435664
H	-0.268235	-2.702051	1.222663
H	-1.669760	-2.138284	2.123007
H	-0.090816	-2.228071	2.909025
H	-3.599103	1.348464	0.077414
H	-3.460968	0.003810	1.197168
H	-4.797595	0.048860	0.040438
H	0.124326	-3.011972	-1.555291
H	1.414640	-2.278515	-0.595643
H	1.666418	-2.589904	-2.308756
C	2.866123	0.625036	-0.018877
O	2.380838	1.080447	-1.062026

CHTS1			
Li	-0.782417	0.491697	-0.249618
N	-2.785327	1.028639	-0.567085
N	-0.216899	-1.074444	-1.490111
N	0.572217	1.995912	-0.725829
N	-0.440727	0.024668	1.724664
H	-3.041018	1.677573	0.166420
C	-3.681740	-0.132092	-0.552989
H	-2.880274	1.534616	-1.438424
H	0.769029	-0.793894	-1.517385
H	-0.554481	-1.030238	-2.443516
C	-0.295999	-2.455297	-1.002215
H	0.519485	-0.293375	1.536093
C	-1.172126	-0.999842	2.470893
H	-0.347576	0.853643	2.298296
H	1.330772	1.348265	-0.966101
C	1.036273	2.896323	0.333248
H	0.374307	2.529874	-1.562640
H	0.219694	3.529803	0.679742
H	1.860994	3.542239	0.024072
H	1.385111	2.301417	1.174798
H	-1.266887	-1.895582	1.860192
H	-2.178282	-0.651400	2.704926
H	-0.687427	-1.286171	3.407101
H	-3.569144	-0.659646	0.391544
H	-3.392021	-0.816926	-1.346775
H	-4.735592	0.122567	-0.683087
H	-1.335458	-2.747323	-0.851936
H	0.219442	-2.516907	-0.046651
H	0.167278	-3.179303	-1.676183
C	2.866262	-0.579634	-0.026716
O	2.522019	-0.122620	-1.132488

O	2.341745	-0.102867	1.223108

CHp1

O	2.419146	-0.079382	0.884597
H	4.381253	-0.805099	3.319460
H	3.967572	-0.612501	2.725294

OHTS1

O	2.210803	-0.776766	1.001083
H	4.032497	-0.879654	0.047018
H	5.173359	-1.169766	0.117786

OHp1

Li	-0.830873	-0.028635	-0.424583
N	-2.850050	-0.277607	-0.929345
N	0.425380	-1.144704	-1.638284
N	-0.134093	1.911535	-0.666208
N	-0.551638	-0.496862	1.554322
H	-2.999028	-0.092083	-1.912865
C	-3.735060	0.556816	-0.111826
H	-3.061375	-1.257573	-0.789461
H	1.214272	-0.499774	-1.506436
H	0.212055	-1.144264	-2.627753
C	0.845244	-2.486694	-1.224371
H	0.472501	-0.410361	1.468664
C	-0.907205	-1.790239	2.136420
H	-0.839899	0.244472	2.180354
H	0.836306	1.605687	-0.816275
C	-0.168587	2.829477	0.474526
H	-0.416672	2.400770	-1.505947
H	-1.197234	3.084693	0.730572
H	0.379527	3.758730	0.302049
H	0.282859	2.339172	1.334592
H	-0.576607	-2.588770	1.475027
H	-1.989592	-1.875858	2.240402
H	-0.459252	-1.966422	3.117434
H	-3.491408	1.604273	-0.276216
H	-3.557785	0.340059	0.939317
H	-4.797316	0.412362	-0.320341
H	-0.001183	-3.173825	-1.237834
H	1.228580	-2.432298	-0.208116
H	1.633671	-2.906789	-1.853455
C	2.901112	0.356938	0.232178
O	2.492568	0.744549	-0.889481
O	2.238549	-0.165791	1.146133
H	3.989021	0.497677	0.426543
H	5.942024	0.771635	0.775322

eTS2

Li	-0.778256	-0.023524	-0.413408
N	-2.743225	-0.653285	-0.762275
N	0.534327	-0.819332	-1.809427
N	-0.474492	2.024813	-0.559392
N	-0.200822	-0.623102	1.474012
H	-2.988522	-0.444586	-1.721893
C	-3.733879	-0.074243	0.150989
H	-2.744644	-1.662812	-0.684802
H	1.280427	-0.161227	-1.585601
H	0.298728	-0.659351	-2.781085
C	1.041043	-2.185784	-1.640218
H	0.820141	-0.557341	1.385347
C	-0.564347	-1.959604	1.949584
H	-0.453133	0.060809	2.177132
H	0.531594	1.954840	-0.407167
C	-1.054429	2.977674	0.390605
H	-0.565978	2.391863	-1.499507
H	-2.122004	3.087874	0.205022
H	-0.596055	3.967433	0.345769
H	-0.933203	2.599945	1.404450
H	-0.271412	-2.700033	1.207302
H	-1.643963	-2.033441	2.082677
H	-0.088282	-2.231161	2.894212
H	-3.730019	1.008080	0.044376
H	-3.453403	-0.304063	1.176718
H	-4.751144	-0.433664	-0.016339
H	0.234913	-2.906115	-1.777186
H	1.429955	-2.294670	-0.630408
H	1.845028	-2.438052	-2.334540
C	3.097387	0.514057	0.455860
O	2.372304	1.103451	-0.435611
O	2.697432	-0.372740	1.196328
H	4.136283	0.865062	0.511227
H	3.016400	1.979245	-1.082573

rFA

Li	0.698653	-0.015093	0.281346
N	2.632336	-0.784004	0.603494
N	-0.325620	-0.336961	2.063560
N	0.836714	2.037098	-0.021380
N	-0.162670	-0.953847	-1.367817
H	2.996644	-0.183555	1.334069
C	3.566562	-0.829119	-0.525427
H	2.540481	-1.702877	1.019330
H	-0.886198	0.515112	2.143904
H	0.288509	-0.301410	2.871337
C	-1.206695	-1.507450	2.173328
H	-1.140855	-0.667006	-1.355571
C	-0.087821	-2.414029	-1.469228
H	0.229797	-0.536765	-2.203479
H	0.137923	2.230991	-0.731168
C	2.067529	2.776098	-0.316075
H	0.419685	2.405453	0.835389
H	2.800559	2.592302	0.468165
H	1.917913	3.855373	-0.387112
H	2.490638	2.429343	-1.257529
H	-0.542254	-2.859610	-0.586858
H	0.953220	-2.733283	-1.502278
H	-0.595487	-2.817316	-2.347840
H	3.668928	0.168538	-0.945996
H	3.163033	-1.475258	-1.302412
H	4.561294	-1.193240	-0.260557
H	-0.612202	-2.419339	2.142714
H	-1.890119	-1.526934	1.326906
H	-1.801123	-1.516486	3.088776
C	-3.192019	0.742534	-0.375442
O	-2.124364	1.471536	-0.095571
O	-3.144470	-0.188863	-1.134586
H	-4.108735	1.052398	0.137547
H	-2.287590	2.123251	0.641956

H_2r2

Li	-0.709943	0.396283	-0.262869
N	-2.714871	0.889428	-0.622922
N	-0.180206	0.295388	1.729479
N	-0.292345	-1.433536	-1.138886
N	0.477722	1.809193	-1.198778
C	3.084006	-0.303866	-0.092398
O	2.693104	-1.579019	-0.369854
O	2.596187	0.297423	0.848706
H	3.961980	0.033040	-0.639847
H	3.097294	-1.852498	-1.209931
H	0.827262	0.244027	1.560634
C	-0.604467	-0.847680	2.540126
H	-0.336075	1.154419	2.241623
C	0.924823	2.969868	-0.416980
H	0.081807	2.120445	-2.080050
H	1.295678	1.258333	-1.473240
H	0.560695	-1.727401	-0.671688
H	0.011084	-1.205999	-2.083179
C	-1.256909	-2.534477	-1.179935
H	-2.793092	1.898835	-0.601295
C	-3.727517	0.282532	0.246557
H	-2.871669	0.619537	-1.587006
H	-3.631198	-0.800395	0.208738
H	-4.753083	0.545766	-0.020385
H	-3.550490	0.592902	1.274080
H	1.576256	3.642334	-0.978628
H	1.476372	2.615501	0.450141
H	0.063338	3.540763	-0.072055
H	-0.378418	-1.768926	2.006748
H	-1.681145	-0.815206	2.703842

Li	-0.738201	0.034018	0.191976
N	0.100591	-1.257070	-1.185575
N	-0.030135	1.924318	-0.234583
N	-2.831566	-0.032427	0.111739
N	-0.002138	-0.458390	2.066038
C	2.856350	-0.122806	-0.299707
O	2.659647	0.483199	-1.591294
O	2.198178	0.448177	0.640295
H	3.918203	-0.369508	-0.145084
H	3.294798	0.091266	-2.195998
C	-0.378307	3.109595	0.543825
H	0.055878	2.167248	-1.213343
H	0.902335	1.571612	0.038401
C	0.006003	-1.827558	2.576755
H	-0.203300	0.185276	2.820448
H	0.932592	-0.205577	1.704914
H	-3.158855	0.566411	0.858970
H	-3.160431	-0.964739	0.327292
C	-3.364748	0.417587	-1.176154
H	0.226450	-0.748572	-2.052426
C	-0.394299	-2.604082	-1.458394
H	1.048192	-1.291660	-0.795621
H	-3.003233	-0.241297	-1.963045
H	-2.988238	1.416031	-1.387099
H	-4.455918	0.440773	-1.221134
H	-0.406751	2.852532	1.602178
H	-1.369215	3.473445	0.268324
H	0.328271	3.935533	0.426632
H	-0.496777	-3.152711	-0.523173
H	0.254863	-3.187279	-2.116836

Li	-0.806338	0.089745	0.219748
N	-0.215651	-1.381020	-1.105131
N	0.022001	1.860442	-0.437845
N	-2.893644	0.217430	0.337193
N	0.077810	-0.309467	2.049427
C	2.706841	-0.430222	-0.586125
O	2.417496	0.090482	-1.895612
O	2.219958	0.276640	0.367416
H	3.750969	-0.774365	-0.525435
H	2.945424	-0.403012	-2.528500
C	-0.158318	3.133489	0.254797
H	0.034540	2.011014	-1.438660
H	0.945924	1.455862	-0.216382
C	0.023363	-1.625338	2.683418
H	0.003896	0.411439	2.755755
H	0.991290	-0.173320	1.587277
H	-3.094003	0.905574	1.051672
H	-3.280717	-0.657477	0.666759
C	-3.508662	0.606230	-0.934277
H	-0.141341	-0.961338	-2.023885
C	-0.841966	-2.697387	-1.201242
H	0.761348	-1.466175	-0.806660
H	4.087771	1.080866	1.543499
H	4.715534	1.301056	1.892463
H	-3.284671	-0.148181	-1.685728
H	-3.069073	1.542839	-1.269943
H	-4.592737	0.729685	-0.883248
H	-0.107748	2.971087	1.330903
H	-1.139241	3.556076	0.032875
H	0.596405	3.882387	0.001031

H	-0.112663	-0.899240	3.514106
H	-2.143379	-2.226902	-1.733747
H	-1.569837	-2.786905	-0.167997
H	-0.866938	-3.440087	-1.649545

CHTS2

C	2.797093	-0.307362	-0.882514
H	2.378778	0.024521	-1.928739
H	1.782861	0.566468	-3.025499
Li	-0.746037	0.184183	0.183194
N	0.034936	1.969597	-0.519267
N	0.480943	-0.333437	1.771382
N	-2.822842	0.153206	0.516237
N	-0.462415	-1.245640	-1.294996
O	2.761867	0.960493	-0.085333
O	2.084407	-1.248573	-0.314303
H	3.879882	-0.537468	-1.048583
H	3.549967	1.467629	-0.340064
C	0.155091	-1.423255	2.706269
H	0.929130	0.427205	2.289593
H	1.224759	-0.668340	1.115548
H	-0.484358	-0.971633	-2.280807
C	-1.052652	-2.587000	-1.157758
H	0.561174	-1.313029	-1.042742
C	-3.490894	0.591308	-0.726719
H	-3.206227	0.669537	1.312096
H	-3.060605	-0.826611	0.695896
H	1.033199	1.702628	-0.476150
C	-0.160207	3.166920	0.317402
H	-0.134460	2.209290	-1.499469
H	-0.237197	-2.279185	2.133867
H	-0.629491	-1.106214	3.413242
H	1.020953	-1.785446	3.289762
H	-3.072907	0.018101	-1.567545
H	-3.258726	1.653174	-0.899430
H	-4.587957	0.467567	-0.720757
H	-2.135814	-2.561952	-1.371936
H	-0.925774	-2.925895	-0.116610
H	-0.593318	-3.351429	-1.810646
H	-1.217126	3.478353	0.289567
H	0.461452	4.031772	0.022667
H	0.084786	2.913309	1.360673

OHp2

Li	0.852163	-0.025984	-0.270139
N	-0.312103	-1.244183	-1.474786
N	0.097607	-0.033016	1.657317
N	2.827505	-0.734867	-0.316593
N	0.803622	1.878769	-1.072080
C	-3.639744	0.423181	0.257985
O	-3.062881	-0.088764	-0.914323
O	-2.697491	1.019517	1.113808
H	-2.890916	0.654030	-1.519790
H	0.536155	0.690538	2.214665
C	0.078823	-1.291308	2.407339
H	-0.859916	0.284155	1.503282
H	0.802163	1.804145	-2.087869
C	1.775777	2.905450	-0.670130
H	-0.140670	2.220078	-0.865290
H	2.826745	-1.746511	-0.357614
C	3.713283	-0.271288	0.756124
H	3.171545	-0.417152	-1.215108
H	-1.258974	-1.013982	-1.175684
C	-0.140115	-2.697675	-1.527116
H	-0.238718	-0.858853	-2.411249
H	-4.065198	-0.418759	0.795783
H	-4.421919	1.142042	0.007480
H	-2.475205	1.896750	0.754965
H	0.850593	-2.941384	-1.909724

H	-1.381426	-2.555776	-1.918438
H	0.296955	-2.506955	1.777483
H	-0.990286	-2.118219	2.911753
H	0.700626	-1.982324	3.406581

CHp2

Li	0.810724	-0.177277	-0.341133
N	-0.515001	-1.409671	-1.363427
N	0.475169	-0.028420	1.690120
N	2.789578	-0.763073	-0.744466
N	0.363944	1.719209	-1.015797
C	-2.948088	0.412336	0.570374
O	-3.121770	-0.094233	-0.788868
O	-1.842796	1.162998	0.706508
H	-3.281735	0.683849	-1.332052
H	1.040371	0.676961	2.146426
C	0.294648	-1.162408	2.594884
H	-0.437130	0.423636	1.488821
H	0.157508	1.827403	-2.000809
C	1.066015	2.912015	-0.539716
H	-0.547929	1.653862	-0.540927
H	2.880387	-1.765177	-0.636156
C	3.756265	-0.069466	0.112327
H	2.977888	-0.562614	-1.718426
H	-1.404521	-0.933252	-1.181522
C	-0.651680	-2.830603	-1.035417
H	-0.356069	-1.313069	-2.359232
H	-2.916930	-0.506975	1.173378
H	-3.867603	0.959409	0.820813
H	-2.326979	2.669853	0.123431
H	0.279182	-3.357779	-1.244175
H	-1.455346	-3.329249	-1.581904
H	-0.858532	-2.937011	0.027327
H	1.269700	2.810349	0.525141
H	0.494227	3.832205	-0.675708
H	2.022296	3.020284	-1.052382
H	-0.360884	-1.895982	2.129050
H	-0.147898	-0.889409	3.556376
H	1.248399	-1.653848	2.790426
H	3.541819	-0.303732	1.152469
H	3.638914	1.004686	-0.013329
H	4.796445	-0.330252	-0.094479

H	-0.890971	-3.152394	-0.213033
H	-0.312858	-3.390130	-1.860832
H	-1.864164	-2.601019	-1.567445
H	0.179665	-2.394132	1.928765
H	-0.956534	-1.795092	3.130758
H	0.779504	-1.769790	3.459383

OHTS2

Li	0.808004	-0.166072	-0.347089
N	-0.530913	-1.385325	-1.366519
N	0.489745	-0.032687	1.688641
N	2.779406	-0.769554	-0.761912
N	0.383460	1.739111	-1.012381
C	-3.000791	0.425388	0.569250
O	-3.156711	-0.089831	-0.783544
O	-1.865736	1.137796	0.725128
H	-3.322879	0.679965	-1.336547
H	1.048537	0.681268	2.139587
C	0.346475	-1.175855	2.588656
H	-0.432287	0.401558	1.506697
H	0.185378	1.851089	-1.998821
C	1.113147	2.915679	-0.535159
H	-0.532069	1.701307	-0.548193
H	2.855344	-1.774544	-0.669680
C	3.757584	-0.104780	0.104878
H	2.970811	-0.556974	-1.732733
H	-1.418068	-0.909590	-1.174157
C	-0.667216	-2.807708	-1.043996
H	-0.381501	-1.284427	-2.363401
H	-3.016199	-0.479058	1.189942
H	-3.897267	1.020018	0.789991
H	-2.235229	2.549835	0.306038
H	0.260779	-3.335437	-1.263677
H	-1.476635	-3.302176	-1.585641
H	-0.864782	-2.918713	0.020059
H	1.314739	2.809021	0.529482
H	0.562074	3.848118	-0.670790
H	2.071014	3.000048	-1.049035
H	-0.305819	-1.917152	2.130555
H	-0.080596	-0.917043	3.560892
H	1.312251	-1.652094	2.760861
H	3.539802	-0.351263	1.141492
H	3.657864	0.972931	-0.004320
H	4.793226	-0.379352	-0.106578

H	-0.876137	-3.202510	-2.156474		
H	-0.217426	-3.112167	-0.523241		
H	1.750237	3.028249	0.411337		
H	1.582523	3.879285	-1.123692		
H	2.780540	2.592270	-0.950381		
H	-0.441346	-2.049290	1.824771		
H	-0.417605	-1.215426	3.377204		
H	1.095947	-1.644420	2.573943		
H	3.335959	-0.626149	1.712877		
H	3.706452	0.816083	0.782421		
H	4.747105	-0.606176	0.649711		

Table S3. Cartesian Coordinates (Å) for the reactants, products, and intermediates of the $Li(NH_2CH_2CH_3)_4 + CO_2 + 2H_2 \rightarrow Li(NH_2CH_2CH_3)_4 + CH_2(OH)_2$ reaction pathway.

$Li(NH_2CH_2CH_3)_4$				CO_2r				eTS1			
Li	0.082002	-0.321862	-0.391258	Li	0.520726	0.379080	-0.302331	Li	-0.574631	-0.002202	-0.405524
N	0.336960	1.745350	-0.486802	N	-0.372371	-0.257296	1.470432	C	3.576261	1.036691	0.412723
N	-1.044876	-0.993179	-1.995223	N	-0.208824	-0.658715	-1.943243	O	4.320125	1.914653	0.288205
N	1.919654	-1.227546	-0.693749	N	-0.074728	2.336502	-0.640621	O	2.968723	0.068524	0.664994
N	-0.687670	-1.020585	1.406571	N	2.605488	0.389258	-0.291561	N	-2.415661	-0.886314	-0.847837
H	1.020223	1.828265	-1.234911	H	-0.762569	0.589594	1.873107	N	0.825058	-0.756218	-1.734270
C	0.804270	2.467489	0.702318	C	0.364399	-1.002094	2.496959	N	-0.569666	2.040347	-0.716728
H	-0.509583	2.174788	-0.843624	H	-1.176877	-0.792223	1.158434	N	-0.007539	-0.409852	1.546930
H	-0.791877	-1.982906	-2.008452	H	-0.037422	-0.023015	-2.721109	H	-2.584242	-0.643871	-1.818792
H	-0.575468	-0.603736	-2.813121	H	-1.217148	-0.611973	-1.800978	C	-3.573754	-0.507297	-0.029623
C	-2.501173	-0.865299	-2.162022	C	0.162809	-2.026119	-2.338754	H	-2.294606	-1.893064	-0.830220
H	-0.746480	-2.014771	1.194475	H	2.786430	0.775654	-1.214514	H	1.584220	-0.081041	-1.625249
C	-1.985421	-0.536806	1.893984	C	3.362671	-0.856115	-0.115015	H	0.501687	-0.627306	-2.689313
H	0.006693	-0.944133	2.142957	H	2.935135	1.088183	0.365652	C	1.357512	-2.116110	-1.571743
H	1.704873	-2.225641	-0.666060	H	0.161341	2.541167	-1.611556	H	0.985993	-0.204475	1.479473
C	3.076841	-0.949838	0.169989	C	0.395094	3.433816	0.218520	C	-0.201873	-1.751877	2.106285
H	2.169486	-1.046644	-1.665991	H	-1.095492	2.307251	-0.628881	H	-0.385422	0.284087	2.182585
H	3.285056	0.119109	0.115411	H	0.130275	3.189482	1.247877	H	0.429796	2.240543	-0.615419
C	4.330838	-1.737363	-0.172715	C	-0.152290	4.805027	-0.142585	C	-1.339279	2.972597	0.119378
H	2.781005	-1.155821	1.199287	H	1.484736	3.448329	0.174886	H	-0.765416	2.222265	-1.698824
H	-2.705687	-0.660072	1.085516	H	2.977483	-1.578738	-0.834014	H	-2.394126	2.706913	0.042143
H	-1.897622	0.536262	2.067626	H	3.127209	-1.249166	0.874035	C	-1.147692	4.440196	-0.225656
C	-2.491691	-1.227067	3.149223	C	4.866635	-0.713939	-0.275580	H	-1.050613	2.798323	1.156443
H	1.709735	1.972561	1.053361	H	1.223063	-0.398831	2.794382	H	0.223211	-2.467158	1.402014
H	0.057626	2.333450	1.485418	H	0.766317	-1.901665	2.030022	H	-1.274148	-1.951623	2.140087
C	1.070982	3.947462	0.485852	C	-0.454249	-1.377324	3.720988	C	0.407271	-1.959530	3.482933
C	-2.954606	0.577258	-2.050403	C	-0.044558	-3.006538	-1.201409	H	-3.677617	0.575480	-0.092013
H	-2.976338	-1.463418	-1.385056	H	1.212279	-2.013791	-2.633075	H	-3.332502	-0.733413	1.009295
H	-2.830560	-1.279298	-3.118687	H	-0.403314	-2.355948	-3.214096	C	-4.878055	-1.180267	-0.421325
H	1.837434	4.098819	-0.274496	H	-0.843588	-0.488024	4.217478	H	0.519657	-2.815149	-1.595617
H	1.413075	4.420163	1.406690	H	0.151228	-1.926902	4.442090	H	1.791233	-2.177148	-0.574459
H	0.167926	4.464305	0.159184	H	-1.302252	-2.004343	3.445246	C	2.395194	-2.517648	-2.606637
H	4.658040	-1.524698	-1.190347	H	-1.240079	4.817828	-0.079495	H	-5.148919	-0.938915	-1.449570
H	4.148851	-2.809230	-0.098043	H	0.125872	5.079500	-1.159988	H	-5.693492	-0.855599	0.224911
H	5.146113	-1.482993	0.506301	H	0.236690	5.567886	0.533613	H	-4.799003	-2.265084	-0.340510
H	-2.477342	1.198223	-2.808920	H	-1.088554	-3.025993	-0.889477	H	-1.451545	4.642403	-1.253129
H	-2.711947	0.989664	-1.070824	H	0.560661	-2.735826	-0.336254	H	-0.101630	4.727370	-0.124324
H	-4.032982	0.652766	-2.190992	H	0.231974	-4.015153	-1.507829	H	-1.741289	5.075101	0.433579
H	-2.614701	-2.297106	2.982018	H	5.119665	-0.348133	-1.271001	H	1.483503	-1.790236	3.459144
H	-3.456040	-0.820399	3.454894	H	5.365784	-1.672498	-0.133176	H	0.231568	-2.974910	3.839020
H	-1.794237	-1.095226	3.977216	H	5.274077	-0.012446	0.453375	H	-0.024566	-1.269804	4.209148
				C	-4.126609	-0.512288	-0.325434	H	1.980266	-2.474951	-3.614441
				O	-5.114673	0.023454	-0.581576	H	2.747564	-3.534615	-2.429727
				O	-3.154761	-1.088734	-0.050793	H	3.254688	-1.849204	-2.569924

CO_2p				H_2r1				CHTS1			
Li	-0.432173	0.170549	-0.491934	Li	-0.381361	0.214579	-0.480686	Li	-0.542896	0.152622	-0.498090
N	-2.475662	0.419406	-0.883154	N	-2.397747	0.637738	-0.859602	N	-2.603169	0.246058	-0.862606
N	0.466011	-1.100859	-1.877261	N	0.430335	-1.083538	-1.895016	N	0.463432	-1.037237	-1.881121
N	0.650581	1.936219	-0.709750	N	0.815389	1.912200	-0.676224	N	0.425629	1.982796	-0.720791
N	-0.122038	-0.464424	1.439284	N	-0.084793	-0.471326	1.435923	N	-0.145797	-0.463446	1.421031
H	-2.599212	0.790529	-1.817995	H	-2.482007	0.999427	-1.802512	H	-2.771760	0.628784	-1.785679
C	-3.166466	1.271067	0.091375	C	-2.983060	1.584723	0.095838	C	-3.342806	1.016792	0.143426
H	-2.889066	-0.505944	-0.892427	H	-2.914961	-0.233636	-0.845292	H	-2.943684	-0.708225	-0.889563
H	1.399405	-0.692551	-1.758995	H	1.387719	-0.735112	-1.777540	H	1.359717	-0.560897	-1.735275
H	0.203470	-0.933363	-2.842053	H	0.172128	-0.883041	-2.854719	H	0.208540	-0.876501	-2.848999
C	0.542994	-2.547798	-1.642169	C	0.421528	-2.536809	-1.687346	C	0.644570	-2.477274	-1.661726
H	0.893150	-0.574350	1.310072	H	0.919209	-0.641768	1.285166	H	0.872764	-0.506081	1.271903
C	-0.671743	-1.694524	2.014352	C	-0.695883	-1.673959	2.007125	C	-0.596222	-1.731332	2.001341
H	-0.236853	0.292666	2.103683	H	-0.138710	0.281041	2.113261	H	-0.297377	0.279459	2.094012
H	1.521589	1.465883	-0.979585	H	1.650636	1.392527	-0.967620	H	1.336828	1.556124	-0.925518
C	0.924054	2.771429	0.465439	C	1.158247	2.702167	0.511992	C	0.579226	2.888056	0.422885
H	0.392179	2.530809	-1.488998	H	0.587044	2.539307	-1.439241	H	0.173088	2.522383	-1.540929
H	-0.017790	3.193893	0.822247	H	0.250830	3.176992	0.891533	H	-0.404465	3.272158	0.701268
C	1.933589	3.880684	0.220403	C	2.234582	3.748715	0.275575	C	1.539026	4.041696	0.181746

H	1.294286	2.112632	1.250637
H	-0.512075	-2.496256	1.293387
H	-1.753700	-1.581193	2.115865
C	-0.062215	-2.085087	3.351151
H	-2.674549	2.243736	0.082580
H	-2.988917	0.845935	1.079000
C	-4.657573	1.435679	-0.148220
C	-0.820747	-3.201683	-1.746772
H	0.959976	-2.691350	-0.646331
H	1.233602	-3.032311	-2.338530
H	-4.850937	1.884073	-1.123494
H	-5.105701	2.078371	0.609340
H	-5.168332	0.472631	-0.113936
H	1.579139	4.569431	-0.548574
H	2.884123	3.463532	-0.110035
H	2.111479	4.456833	1.128773
H	-1.253728	-3.051104	-2.737520
H	-1.510454	-2.786859	-1.011090
H	-0.752370	-4.275623	-1.577223
H	1.014946	-2.215290	3.253697
H	-0.489928	-3.017193	3.721781
H	-0.241283	-1.313084	4.101267
C	3.309234	-0.303088	-0.079437
O	2.981205	0.232645	-1.147069
O	2.673177	-0.787471	0.853282

CHp1

H	1.495270	2.003812	1.277708
H	-0.623503	-2.467427	1.263033
H	-1.761591	-1.486332	2.157812
C	-0.061054	-2.138220	3.308116
H	-2.371762	2.487087	0.079809
H	-2.870056	1.154826	1.090891
C	-4.438983	1.933861	-0.161820
C	-0.977745	-3.106932	-1.808675
H	0.825613	-2.723538	-0.693344
H	1.085478	-3.047466	-2.390910
H	-4.564853	2.387858	-1.145571
H	-4.808008	2.640552	0.581297
H	-5.068354	1.044385	-0.118992
H	1.915750	4.475726	-0.473536
H	3.151495	3.278093	-0.077264
H	2.461513	4.292092	1.193167
H	-1.394736	-2.916840	-2.799495
H	-1.646912	-2.661758	-1.072078
H	-0.974185	-4.185372	-1.654590
H	0.999783	-2.338210	3.162135
H	-0.536351	-3.048212	3.675756
H	-0.155931	-1.374676	4.081815
C	3.335173	-0.498941	-0.116127
O	3.032869	0.077885	-1.169696
O	2.677215	-0.961738	0.812490
H	-4.537490	-1.961443	0.312522
H	-3.888762	-2.074953	0.662875

OHTS1

H	0.933460	2.291855	1.263803
H	-0.413990	-2.514925	1.265770
H	-1.678588	-1.687572	2.144069
C	0.087526	-2.094856	3.309549
H	-2.927866	2.024676	0.153861
H	-3.117715	0.581972	1.116988
C	-4.845554	1.071169	-0.072200
C	-0.665475	-3.229345	-1.790072
H	1.059458	-2.602017	-0.662518
H	1.376754	-2.901098	-2.355337
H	-5.087822	1.528860	-1.032118
H	-5.330518	1.656869	0.708505
H	-5.279792	0.070808	-0.057710
H	1.193276	4.672156	-0.639234
H	2.529278	3.666970	-0.074716
H	1.630337	4.668774	1.068970
H	-1.098334	-3.097656	-2.783505
H	-1.391530	-2.876923	-1.056840
H	-0.518939	-4.297412	-1.633584
H	1.166409	-2.151442	3.169868
H	-0.263443	-3.057173	3.683612
H	-0.113730	-1.344381	4.075732
C	3.279694	-0.119693	-0.064907
O	2.872040	0.449090	-1.095073
O	2.656550	-0.656469	0.856135
H	4.477056	-0.151239	0.044106
H	5.661967	-0.175624	0.148996

OHp1

Li	-0.495792	0.091458	-0.524246
N	-2.554540	0.002909	-0.905050
N	0.632143	-1.008854	-1.882955
N	0.319634	1.992238	-0.740267
N	-0.070413	-0.478089	1.399535
H	-2.744900	0.261520	-1.866066
C	-3.350824	0.829926	0.007742
H	-2.822720	-0.970549	-0.817849
H	1.475319	-0.448590	-1.705826
H	0.394140	-0.870587	-2.858474
C	0.941220	-2.424560	-1.655444
H	0.949479	-0.423282	1.240871
C	-0.389208	-1.780811	1.987431
H	-0.289276	0.248667	2.071751
H	1.264969	1.623175	-0.913347
C	0.378079	2.916913	0.395087
H	0.054582	2.503882	-1.574175
H	-0.636711	3.233400	0.646497
C	1.259190	4.134264	0.164384
H	0.753332	2.356210	1.251228
H	-0.152106	-2.545533	1.247457
H	-1.467647	-1.838148	2.155818
C	0.356038	-2.078271	3.278930
H	-3.011676	1.859799	-0.103665
H	-3.095364	0.531545	1.024548
C	-4.853391	0.747035	-0.200927
C	-0.289516	-3.297015	-1.807866
H	1.345683	-2.507595	-0.647680
H	1.724193	-2.780195	-2.332318
H	-5.128152	1.068735	-1.206276
H	-5.381493	1.383342	0.509076
H	-5.211913	-0.274049	-0.065243
H	0.888824	4.731389	-0.670778
H	2.278591	3.827577	-0.066993
H	1.285492	4.774262	1.046897
H	-0.711933	-3.208679	-2.810608
H	-1.060888	-3.011456	-1.092012
H	-0.047455	-4.346499	-1.643309
H	1.431446	-2.026842	3.113034
H	0.109617	-3.070839	3.657927
H	0.099604	-1.351463	4.051715

Li

Li	-0.532799	0.177195	0.050172
N	-2.508647	0.008149	0.721390
N	-0.159637	-0.741761	-1.777983
N	-0.015155	2.157117	-0.316652
N	0.773712	-0.561687	1.462987
H	-2.643115	-0.924692	1.094429
C	-3.535620	0.295350	-0.287605
H	-2.611758	0.639926	1.507456
H	0.706287	-0.224960	-1.932452
H	-0.784459	-0.470967	-2.529205
C	0.117686	-2.181343	-1.870552
H	1.636197	-0.589667	0.905534
C	0.569548	-1.877564	2.078339
H	0.946371	0.118646	2.194904
H	0.903165	1.943809	-0.706931
C	0.127790	3.121115	0.779684
H	-0.529354	2.590167	-1.076221
H	-0.856811	3.289443	1.220717
C	0.748626	4.447613	0.374627
H	0.736262	2.651582	1.553518
H	0.386927	-2.592943	1.275750
H	-0.343141	-1.844792	2.677630
C	1.734339	-2.354999	2.930204
H	-3.383789	-0.398383	-1.113960
H	-3.338763	1.292533	-0.681391
C	-4.965872	0.205142	0.215748
C	-1.124069	-3.003268	-1.588512
H	0.896636	-2.409883	-1.144269
H	0.519471	-2.450871	-2.851213
H	-5.187921	-0.795854	0.587419
H	-5.674123	0.429894	-0.581373
H	-5.141483	0.912167	1.027431
H	0.135128	4.952498	-0.372636
H	1.737447	4.295453	-0.056645
H	0.846527	5.112287	1.233388
H	-1.915184	-2.778608	-2.306049
H	-1.508727	-2.799698	-0.588807
H	-0.909377	-4.068793	-1.658588
H	2.646503	-2.398038	2.336349
H	1.541627	-3.346984	3.339706
H	1.909006	-1.675948	3.766166

OHTS1

Li	0.381081	0.038615	0.353591
N	2.085619	-1.195846	0.518872
N	-0.584230	-0.028381	2.199736
N	1.053202	1.994559	0.084236
N	-0.743137	-0.538002	-1.307234
H	2.718057	-0.655785	1.099341
C	2.770516	-1.616507	-0.708151
H	1.828335	-2.007224	1.069262
H	-0.970367	0.919305	2.253635
H	0.093652	-0.051182	2.957229
C	-1.649101	-1.001428	2.484622
H	-1.525385	0.116337	-1.322597
C	-1.281124	-1.898951	-1.425908
H	-0.195042	-0.326055	-2.134209
H	0.480679	2.366504	-0.667134
C	2.458268	2.357147	-0.125182
H	0.701127	2.468126	0.918790
H	3.022444	2.006294	0.740637
C	2.707573	3.842791	-0.327193
H	2.830509	1.798433	-0.985638
H	-1.893006	-2.086684	-0.544076
H	-0.448812	-2.603984	-1.381645
C	-2.104294	-2.138575	-2.680290
H	3.006922	-0.717454	-1.277238
H	2.055791	-2.181490	-1.306736
C	4.029185	-2.438150	-0.487348
C	-1.104485	-2.414773	2.540873
H	-2.393632	-0.921374	1.692646
H	-2.162517	-0.768516	3.421209
H	4.767036	-1.876527	0.086535
H	4.485562	-2.715921	-1.437275
H	3.806998	-3.356030	0.058075
H	2.362591	4.412571	0.534990
H	2.174798	4.211387	-1.204251
H	3.769981	4.044945	-0.468078
H	-0.357461	-2.514968	3.329883
H	-0.640579	-2.695650	1.595192
H	-1.900959	-3.128217	2.749980
H	-2.948884	-1.451615	-2.717981
H	-2.490486	-3.157733	-2.706662
H	-1.502543	-1.985858	-3.577659

C	3.339995	0.137219	-0.043087
O	2.865101	0.676579	-1.073615
O	2.714918	-0.441429	0.864939
H	-2.526171	0.269006	3.680914
H	4.443099	0.180590	0.062692

eTS2

C	3.354023	0.085006	-1.052223
O	2.404187	0.820813	-1.525701
O	3.215904	-0.723631	-0.145682
H	4.330810	0.228643	-1.532659
H	2.796687	1.549948	-2.473923

rFA

C	-3.165343	1.857551	-0.204492
O	-1.946893	2.294569	0.059220
O	-3.377290	1.037634	-1.059699
H	-3.954919	2.295151	0.415760
H	-1.917015	2.868797	0.880228

H_2r2

Li	-0.271453	0.322268	-0.252884
N	-1.866015	1.708684	-0.127434
N	-0.241663	-1.023081	-1.851167
N	1.399594	1.520663	-0.635022
H	2.048046	0.781691	-0.911722
C	1.984911	2.300667	0.463488
H	1.306671	2.116175	-1.450686
H	1.260663	3.058635	0.770062
C	3.314440	2.953835	0.128466
H	-0.485766	-0.583776	-2.731877
C	-0.879814	-2.345664	-1.782157
H	0.615623	-1.329785	1.481777
C	-1.331063	-1.284253	2.113295
H	0.236400	0.015256	2.278479
H	2.114535	1.626649	1.308919
H	-1.618273	-2.062842	1.406423
H	-2.143674	-0.555459	2.117761
H	-2.743032	-1.753628	-2.707499
H	-2.745559	-1.647254	-0.946548
H	-2.850927	-3.219789	-1.740389
H	-0.373874	-2.630398	3.504457
H	-2.091342	-2.359047	3.829680
C	-1.166444	-1.883352	3.499885
H	-3.527500	0.524661	0.254522
H	-3.322117	0.981290	-1.415838
C	-4.252720	2.498319	-0.203237
N	-0.126930	-0.628952	1.580430
H	-1.773789	2.047670	0.824245
C	-3.266236	1.359300	-0.395478
H	-1.585538	2.480618	-0.721748
H	0.771395	-1.141234	-1.868564
C	-2.390597	-2.234154	-1.792797
H	-0.543759	-2.822533	-0.861437
H	-0.554234	-2.990417	-2.603421
H	-4.229479	2.867961	0.822547
H	-5.270387	2.172831	-0.417888
H	-4.022090	3.332958	-0.866472
H	3.213993	3.641747	-0.713005
H	4.052458	2.196842	-0.133544
H	3.696460	3.518515	0.979200
H	-0.902686	-1.115489	4.228211
C	3.121435	-1.532851	-0.381130
O	3.587756	-0.719108	0.578132
O	2.701370	-1.069906	-1.430327
H	3.757793	-1.241871	1.388340
H	3.252956	-2.596951	-0.197426

CHTS2

Li	-0.469055	0.056369	-0.510575
N	-2.485913	-0.507503	-0.701270
N	0.726905	-0.858126	-1.932409
N	-0.204110	2.100978	-0.778681
H	0.814961	1.930603	-0.767533
C	-0.546807	3.096861	0.235702
H	-0.420508	2.470645	-1.697068
H	-1.631413	3.226434	0.255764
C	0.130096	4.445554	0.045534
H	0.500738	-0.690294	-2.905508
C	1.254518	-2.215329	-1.781494
H	1.217576	-0.273125	1.236906
C	-0.022841	-1.722461	1.975823
H	-0.061399	0.313429	2.049090
H	-0.267627	2.687277	1.207705
H	0.317898	-2.468917	1.257865
H	-1.100154	-1.868402	2.084762
H	-0.271787	-3.193678	-2.963221
H	-0.615916	-3.150711	-1.233951
H	0.589183	-4.272722	-1.870119
H	1.741944	-1.824545	3.213737
H	0.468252	-2.953311	3.691952
C	0.664467	-1.949676	3.313132
H	-3.286949	1.164035	0.224454
H	-3.057029	-0.213844	1.269435
C	-4.862656	-0.299358	0.100261
N	0.213225	-0.403322	1.386971
H	-2.758203	-0.240719	-1.640108
C	-3.402499	0.081769	0.278584
H	-2.538314	-1.518898	-0.670287
H	1.460430	-0.174190	-1.666345
C	0.178667	-3.268201	-1.971778
H	1.680389	-2.287664	-0.781104
H	2.078263	-2.409230	-2.475693
H	-5.232663	0.014845	-0.876463
H	-5.485234	0.172207	0.860578
H	-4.998400	-1.378708	0.179153
H	-0.159841	4.894895	-0.905637
H	1.213394	4.330741	0.045005
H	-0.142244	5.140423	0.840929
H	0.311783	-1.235303	4.058708
C	3.431586	0.700638	-0.216801
O	3.146083	-0.187000	0.899946
O	2.376127	1.087334	-0.833642
H	3.982361	-0.554095	1.195958
H	4.182064	1.448076	0.086267

CHp2

Li	0.607219	0.227580	-0.381020
N	-0.030268	-0.499786	1.443345
N	0.967859	-1.350739	-1.683972
N	-0.993684	1.232196	-1.246825
N	2.214406	1.563696	-0.169399
H	-0.626354	-1.164150	0.921274
C	-0.859940	0.278550	2.363977
H	0.629598	-1.057646	1.972229
H	0.864217	-1.061363	-2.648706
H	0.048914	-1.727314	-1.388866
C	1.976649	-2.410788	-1.601395
H	2.472510	1.915470	-1.083850
C	3.384910	0.980915	0.494787
H	1.876239	2.360789	0.357161
H	-0.970335	1.138693	-2.255939
C	-1.288200	2.621092	-0.892106
H	-1.756453	0.623200	-0.937477
H	-1.314840	2.686006	0.196382
C	-2.588429	3.161834	-1.466457
H	-0.454177	3.246553	-1.218501
H	3.696907	0.116732	-0.091323
H	3.053609	0.595476	1.458752
C	4.552349	1.934566	0.684950
H	-1.631582	0.768999	1.771105
H	-0.251419	1.068936	2.810983
C	-1.519802	-0.545200	3.458317
C	2.081598	-2.945028	-0.185898
H	2.941045	-2.007709	-1.919394
H	1.744397	-3.240675	-2.276614
H	-2.157349	-1.312800	3.021622
H	-2.134495	0.080285	4.106491
H	-0.770728	-1.038930	4.080225
H	-3.434892	2.567462	-1.124259
H	-2.575167	3.130763	-2.556880
H	-2.753716	4.195907	-1.162250
H	1.114043	-3.317696	0.148983
H	2.401925	-2.162582	0.502716
H	2.802486	-3.760173	-0.131773
H	4.913114	2.308888	-0.273956
H	5.384488	1.437710	1.183574
H	4.262581	2.792408	1.293115
C	-2.583777	-1.841748	-0.883971
O	-3.177580	-0.625923	-0.339025
O	-1.408967	-2.075137	-0.432752
H	-4.034829	-0.522570	-0.761767
H	-3.334831	-2.647378	-0.886917
H	-4.807179	0.629416	2.227802
H	-4.367337	0.260316	1.748071

OHTS2

Li	0.624566	0.395461	-0.451573
C	-2.489942	-1.893297	-0.641074
H	-2.548581	-1.626189	-1.784614
H	-2.555270	-1.131633	-3.036016
N	-0.025682	-0.266766	1.419158
N	0.942686	-1.297646	-1.617922
N	-1.105833	1.243170	-1.238335
N	2.277358	1.686468	-0.274112
H	-0.565592	-1.026655	0.938838
C	-0.978031	0.475389	2.269158
H	0.623274	-0.768602	2.034119
H	0.815048	-1.147059	-2.623330
H	0.023181	-1.667566	-1.261955
C	1.933950	-2.374651	-1.418070

Li	0.342358	0.040573	-0.366567
N	-0.697618	-1.291526	-1.598395
N	0.097659	-0.303071	1.656885
N	2.345128	0.239830	-0.993055
N	-0.647235	1.833859	-0.668852
C	-3.369099	-0.519643	0.575353
O	-3.496775	-0.595690	-0.879534
O	-2.509975	0.432287	0.971786
H	-3.904106	0.233084	-1.148508
H	0.499791	0.434119	2.225349
C	0.258825	-1.580194	2.353537
H	-0.908617	-0.068526	1.558560
H	-0.942750	2.024558	-1.619445
C	-0.235152	3.088247	-0.033720

Li	-0.534747	-0.059812	-0.325228
O	2.124613	1.541679	-0.787917
H	2.272213	1.669855	-2.270755
N	-2.402464	-1.024778	-0.259501
N	0.649633	-0.800018	-1.844389
N	-0.641923	1.979436	-0.640084
H	0.386473	2.025751	-0.634297
C	-1.187660	2.937977	0.320297
H	-0.917608	2.247380	-1.578240
H	-2.275782	2.845514	0.333398
C	-0.795632	4.383770	0.057354
H	0.332697	-0.605415	-2.787468
C	1.287390	-2.117832	-1.811917
H	1.464432	-0.241931	1.075752

H	2.598222	2.090460	-1.160024	H	-1.471629	1.453660	-0.178452	C	0.433914	-1.631227	2.173550
C	3.385451	0.910776	0.325739	H	2.756384	-0.657596	-1.221632	H	0.358882	0.405418	2.069232
H	2.077243	2.493964	0.325202	C	3.204037	0.961533	-0.046729	H	-0.844967	2.643869	1.314145
H	-1.270785	1.131429	-2.244075	H	2.287026	0.753721	-1.864814	H	0.623240	-2.439941	1.466242
C	-1.420263	2.634855	-0.861149	H	-1.656692	-0.970408	-1.433003	H	-0.592670	-1.760453	2.523751
H	-1.810614	0.624714	-0.801052	C	-0.648650	-2.747067	-1.416473	H	-0.226777	-3.131641	-2.978439
H	-1.186904	2.745536	0.212183	H	-0.495155	-1.075985	-2.568535	H	-0.480058	-3.222826	-1.234976
C	-2.872594	3.042119	-1.118083	H	-3.040047	-1.534970	0.842935	H	0.766324	-4.208384	-2.003027
H	-0.731517	3.305753	-1.404206	H	-4.382537	-0.368408	0.972410	H	2.424170	-1.634084	3.010415
H	3.574147	0.049356	-0.336406	H	-3.442730	1.802331	1.123154	H	1.297263	-2.710108	3.844351
H	3.010681	0.496684	1.276526	C	0.756800	-3.286063	-1.597123	C	1.394064	-1.744343	3.347335
C	4.671569	1.704016	0.556146	H	-1.330555	-3.262334	-2.099103	H	-3.588390	0.661149	-0.472102
H	-1.716619	0.942748	1.598288	H	-1.000775	-2.963347	-0.408619	H	-3.338562	0.146211	1.174571
H	-0.439073	1.290606	2.785670	H	-0.020308	2.868758	1.013047	C	-4.884283	-0.944837	0.146484
C	-1.714689	-0.410213	3.275156	C	-1.265912	4.202218	-0.115106	N	0.517027	-0.370088	1.436064
C	1.985559	-2.757561	0.060131	H	0.705764	3.418022	-0.481833	H	-2.544487	-1.363292	-1.204104
H	2.925788	-2.021041	-1.755681	H	-0.234157	-2.349388	1.758616	C	-3.549845	-0.218677	0.169282
H	1.690855	-3.274876	-2.015548	H	-0.240475	-1.577204	3.327653	H	-2.317882	-1.849172	0.323872
H	-2.266459	-1.195192	2.733739	C	1.720438	-1.939925	2.539801	H	1.348207	-0.073963	-1.648427
H	-2.431837	0.172731	3.878331	H	3.230007	0.383674	0.876286	C	0.280095	-3.233283	-2.017113
H	-1.003021	-0.896696	3.965059	H	2.708424	1.902108	0.192504	H	1.775276	-2.222153	-0.843650
H	-3.556426	2.384065	-0.556611	C	4.616075	1.224777	-0.541696	H	2.079350	-2.199673	-2.562541
H	-3.120744	2.951278	-2.189290	H	2.229873	-2.010911	1.578487	H	-5.124077	-1.291409	-0.859450
H	-3.060951	4.083978	-0.808473	H	1.827418	-2.894898	3.053200	H	-5.690937	-0.289637	0.475103
H	0.986132	-3.075865	0.398833	H	2.234661	-1.184771	3.137040	H	-4.869615	-1.813424	0.806114
H	2.296639	-1.894209	0.672178	H	4.607286	1.825977	-1.451772	H	-1.162401	4.714100	-0.915441
H	2.701259	-3.577857	0.231763	H	5.135392	0.290929	-0.760749	H	0.288317	4.492211	0.057423
H	5.062654	2.103981	-0.394763	H	5.197630	1.762242	0.207139	H	-1.209484	5.049376	0.815905
H	5.453460	1.069419	1.004965	H	1.138603	-3.058142	-2.594179	H	1.198324	-0.966038	4.086314
H	4.492538	2.555128	1.234778	H	0.778110	-4.368388	-1.476305	C	3.323476	1.280864	-0.254197
O	-3.021053	-0.668530	0.031743	H	1.436727	-2.850438	-0.864976	O	3.322981	-0.090652	0.276808
O	-1.272189	-2.156645	-0.232635	H	-1.471688	4.463910	-1.154874	H	4.230537	-0.352952	0.455035
H	-3.967477	-0.622825	-0.188834	H	-0.913273	5.101591	0.391409	H	3.561244	1.943617	0.591689
H	-3.252776	-2.695738	-0.477009	H	-2.200372	3.885580	0.347556	H	4.135203	1.336926	-0.996911

OHp2

Li	-0.469055	0.056369	-0.510575
N	-2.485913	-0.507503	-0.701270
N	0.726905	-0.858126	-1.932409
N	-0.204110	2.100978	-0.778681
H	0.814961	1.930603	-0.767533
C	-0.546807	3.096861	0.235702
H	-0.420508	2.470645	-1.697068
H	-1.631413	3.226434	0.255764
C	0.130096	4.445554	0.045534
H	0.500738	-0.690294	-2.905508
C	1.254518	-2.215329	-1.781494
H	1.217576	-0.273125	1.236906
C	-0.022841	-1.722461	1.975823
H	-0.061399	0.313429	2.049090
H	-0.267627	2.687277	1.207705
H	0.317898	-2.468917	1.257865
H	-1.100154	-1.868402	2.084762
H	-0.271787	-3.193678	-2.963221
H	-0.615916	-3.150711	-1.233951
H	0.589183	-4.272722	-1.870119
H	1.741944	-1.824545	3.213737
H	0.468252	-2.953311	3.691952
C	0.664467	-1.949676	3.313132
H	-3.286949	1.164035	0.224454
H	-3.057029	-0.213844	1.269435
C	-4.862656	-0.299358	0.100261
N	0.213225	-0.403322	1.386971
H	-2.758203	-0.240719	-1.640108
C	-3.402499	0.081769	0.278584
H	-2.538314	-1.518898	-0.670287
H	1.460430	-0.174190	-1.666345
C	0.178667	-3.268201	-1.971778
H	1.680389	-2.287664	-0.781104
H	2.078263	-2.409230	-2.475693

H	-5.232663	0.014845	-0.876463		
H	-5.485234	0.172207	0.860578		
H	-4.998400	-1.378708	0.179153		
H	-0.159841	4.894895	-0.905637		
H	1.213394	4.330741	0.045005		
H	-0.142244	5.140423	0.840929		
H	0.311783	-1.235303	4.058708		
C	3.431586	0.700638	-0.216801		
O	3.146083	-0.187000	0.899946		
O	2.376127	1.087334	-0.833642		
H	3.982361	-0.554095	1.195958		
H	4.182064	1.448076	0.086267		

Table S4. Cartesian Coordinates (Å) for the reactants, products, and intermediates of the $Li(H_2O)_4 + CO_2 + 2H_2 \rightarrow Li(H_2O)_4 + CH_2(OH)_2$ reaction pathway.

$Li(H_2O)_4$				CO_2r				eTS1			
Li	0.000560	-0.194855	-0.006648	Li	-1.419941	0.127168	-0.012298	Li	-1.282195	0.192923	0.059348
O	1.026615	1.006907	-1.144121	O	-0.522047	1.808139	-0.221029	O	-0.614643	-0.089939	1.843150
O	-1.572955	-1.070356	-0.702400	O	-2.660465	0.014021	1.473059	O	-0.661779	-1.307243	-1.035224
O	1.567894	-1.106131	0.656081	O	-2.526795	-0.496281	-1.469007	O	-3.163448	-0.209424	-0.170910
O	-1.022291	0.957655	1.185178	O	0.032747	-1.173148	0.207921	O	-0.557957	1.883465	-0.477871
H	0.983959	1.910799	-0.771353	H	0.439306	1.723885	-0.163946	H	-0.095804	0.614627	2.257662
H	0.860917	1.116278	-2.092665	H	-0.766104	2.616390	0.236901	H	-0.116812	-0.908647	2.001275
H	-1.804007	-1.256686	-1.617762	H	-3.521111	-0.285916	1.147097	H	-0.328418	-1.130874	-1.929445
H	-2.277313	-0.515613	-0.340989	H	-2.396156	-0.646786	2.132041	H	0.027071	-1.850239	-0.610645
H	-0.972861	1.877925	0.855679	H	-0.033660	-1.643487	1.059726	H	0.413303	1.850297	-0.478856
H	-0.853943	1.020797	2.137553	H	-0.085494	-1.878570	-0.456705	H	-0.819817	2.411051	-1.239701
H	2.278097	-0.538712	0.327319	H	-2.387531	-0.298202	-2.403951	H	-3.142382	-1.094890	-0.555293
H	1.789355	-1.334817	1.564263	H	-2.633168	-1.462201	-1.413070	H	-3.794758	-0.234944	0.554696
				C	2.763058	0.002353	-0.000235	C	2.437951	-0.108239	-0.062958
				O	3.269571	-1.027304	0.080562	O	2.383966	-1.264261	0.055879
				O	2.290164	1.059483	-0.083979	O	2.248423	1.039186	-0.190023
CO_2p				H_2r1				CHTS1			
Li	1.342405	0.002613	0.001085	Li	-1.452586	0.181478	0.012432	Li	-1.488532	0.000010	0.000014
O	0.278070	1.333320	-0.884002	O	-0.687395	-1.369048	-0.821877	O	-0.410423	1.334324	0.855900
O	2.228056	-1.448336	-0.966983	O	-2.065752	1.730301	-1.009970	O	-2.361495	-1.451296	0.978651
O	2.197767	1.463950	0.981827	O	-2.563218	-1.032012	1.068406	O	-2.361557	1.451343	-0.978530
O	0.281096	-1.339504	0.871533	O	-0.127458	1.322437	0.803601	O	-0.410524	-1.334340	-0.855968
H	-0.713223	1.243050	-0.659748	H	0.305266	-1.464547	-0.614483	H	0.584333	1.228490	0.642817
H	0.317566	1.619821	-1.798226	H	-0.798886	-1.677651	-1.722927	H	-0.455315	1.649506	1.760236
H	2.436212	-1.686548	-1.872211	H	-2.267476	1.966168	-1.917252	H	-2.576065	-1.686430	1.883136
H	1.582984	-2.085121	-0.628857	H	-1.304974	2.254513	-0.724484	H	-1.704233	-2.080898	0.650728
H	-0.709630	-1.252026	0.642983	H	0.820123	1.038372	0.563941	H	0.584233	-1.228559	-0.642924
H	0.315363	-1.626346	1.785905	H	-0.083741	1.653412	1.702588	H	-0.455467	-1.649572	-1.760283
H	1.550477	2.092180	0.632270	H	-2.067374	-1.799342	0.751160	H	-1.704247	2.080908	-0.650630
H	2.386442	1.704368	1.890745	H	-2.793605	-1.184262	1.986692	H	-2.576186	1.686518	-1.882990
C	-2.672577	-0.003949	0.000677	C	2.496558	-0.594854	-0.060920	C	2.566840	-0.000016	-0.000110
O	-2.189438	-1.093518	0.314746	O	2.243583	0.581030	0.213292	O	2.062094	-1.071154	-0.357329
O	-2.190293	1.084897	-0.317142	O	1.802663	-1.579639	-0.315184	O	2.062124	1.071087	0.357230
				H	4.124118	2.231015	0.365364	H	3.844616	0.000196	0.000165
				H	4.625575	2.782465	0.431482	H	4.881140	0.000200	0.000730
CHp1				OHTS1				OHp1			
Li	-1.517215	0.000167	-0.000005	Li	-1.272884	0.260471	0.088888	Li	-1.569269	0.230672	-0.009476
O	-0.427068	1.316435	0.858182	O	-0.517842	-1.588213	0.266406	O	-0.327504	1.681950	0.041301
O	-2.363757	-1.494461	0.957723	O	-0.508191	0.916192	1.755901	O	-3.035478	0.282337	-1.273540
O	-2.362658	1.495414	-0.957762	O	-0.806306	1.602782	-1.185460	O	-0.486196	-1.448695	-0.351128
O	-0.427751	-1.316775	-0.858015	O	-2.967634	-0.635138	-0.317727	O	-2.523676	-0.161045	1.627590
H	0.581820	1.189643	0.639670	H	0.447839	-1.602153	0.028099	H	0.603622	1.405920	-0.010049
H	-0.465982	1.641546	1.758869	H	-0.550059	-1.863923	1.186711	H	-0.400789	2.546126	-0.368781
H	-2.478840	-1.750190	1.874607	H	0.419976	0.843623	1.451100	H	-2.984742	-0.400913	-1.957509
H	-1.669792	-2.052359	0.573458	H	-0.613357	1.819152	2.066328	H	-3.856249	0.104178	-0.795299
H	0.581119	-1.190135	-0.639802	H	-2.590673	-1.505661	-0.494492	H	-2.261163	0.137469	2.506706
H	-0.467039	-1.642135	-1.758592	H	-3.728731	-0.515251	-0.888529	H	-2.671290	-1.120827	1.700973
H	-1.668674	2.052814	-0.572780	H	0.074160	2.041329	-1.021921	H	-0.738578	-1.874646	-1.197463
H	-2.477262	1.751827	-1.874515	H	-0.976611	1.701674	-2.126350	H	-0.770254	-2.100139	0.333130
C	2.560877	-0.000451	0.000047	C	2.361720	-0.184000	-0.412623	C	3.064278	-0.421165	-0.011058
O	2.013339	-1.056921	-0.381922	O	1.798210	0.745395	0.293778	O	1.792313	-0.021613	-0.146294
O	2.013705	1.056347	0.381323	O	2.037067	-1.361293	-0.392189	O	3.964505	0.343567	0.121519
H	3.665420	-0.000922	0.000574	H	3.161750	0.156990	-1.080257	H	3.182228	-1.513375	-0.037406
H	6.019130	0.001814	0.002009	H	1.721590	1.808994	-0.277298	H	1.147636	-0.760828	-0.235117
eTS2				rFA				H_2r2			
Li	1.567421	0.644996	0.106471	Li	-1.406507	0.329770	0.132365	Li	1.628071	-0.126637	0.437149
C	-2.077298	-0.259321	-0.411662	O	-0.423398	-0.253536	1.718517	O	1.061686	1.726614	0.251889
O	-3.161687	0.148855	0.271419	O	-0.709806	-0.772406	-1.396898	O	0.625385	-0.917082	-1.150271
O	-1.378407	-1.158912	0.034644	O	-3.007919	-0.835311	0.082207	O	3.250491	-0.421780	-0.629360
H	-1.972490	0.154896	-1.411430	O	-0.720729	2.107279	-0.098316	O	0.545533	-0.663277	1.940683
H	-3.505858	0.949799	-0.148399	C	2.080942	0.129574	0.274725	C	-2.403444	0.323012	-0.042417
O	0.500039	-0.107404	1.581998	O	2.666896	-1.091023	-0.068145	O	-2.823208	-0.960759	-0.413586
O	0.434526	2.077764	-0.411668	O	1.279148	0.597145	-0.636944	O	-1.118555	0.365039	0.227612

O	3.323506	-0.201393	0.056986
O	0.992652	-1.005770	-1.050080
H	0.168059	0.375557	2.340834
H	-0.286565	-0.569137	1.181720
H	0.420907	2.745747	-1.103788
H	-0.466140	1.657161	-0.414576
H	0.949924	-1.062851	-2.006477
H	0.062436	-1.199468	-0.712500
H	2.861152	-0.993377	-0.260404
H	3.845061	-0.462510	0.819177

CHTS2

H	2.785211	0.828281	0.745387
H	3.249522	-1.365579	0.644011
H	-0.473937	0.274912	2.518858
H	0.531526	-0.214422	1.440042
H	-0.899654	2.811013	-0.722702
H	0.183584	1.721269	-0.317810
H	-3.236931	-1.347238	0.861757
H	-2.457802	-1.407711	-0.472792
H	0.207526	-0.373100	-1.199361
H	-0.828714	-0.711367	-2.346201

CHp2

H	-3.087368	0.822745	0.653286
H	-3.733480	-0.908957	-0.714116
H	-1.886941	3.340033	-1.825679
H	-2.059772	2.667117	-1.547472
H	1.156726	2.420542	0.906236
H	0.093176	1.499727	0.209777
H	0.367338	-1.524020	2.322273
H	-0.287282	-0.362576	1.476164
H	3.845831	0.288315	-0.880096
H	2.641239	-0.555439	-1.371305
H	-0.196524	-0.454197	-0.783402
H	0.352853	-1.821493	-1.318338

OHTS2

C	-2.363575	0.224054	-0.426381
H	-2.651402	-0.243636	-1.563487
H	-2.911461	-0.716717	-2.429061
Li	1.614169	0.214723	0.451963
O	1.225400	1.461637	-1.046672
O	0.600192	-1.419124	-0.285157
O	3.263642	-0.826217	0.007590
O	0.363045	0.922881	1.785232
O	-2.673702	-0.817324	0.491245
O	-1.074279	0.528645	-0.347127
H	-3.052134	1.073423	-0.307912
H	-3.569462	-1.120480	0.300391
H	1.333597	2.414674	-1.006537
H	0.246683	1.309041	-1.032783
H	0.046166	0.511780	2.592732
H	-0.385695	0.831944	1.126740
H	3.931265	-0.519350	-0.611376
H	2.678606	-1.404137	-0.504863
H	-0.176676	-0.782000	-0.413307
H	0.215082	-2.147024	0.210966

OHp2

O	-1.132936	0.344875	-0.031131
O	-3.046022	-0.974527	-0.008248
O	0.754277	1.658125	1.225154
O	3.276631	-0.798675	-0.065345
O	0.667970	-1.384883	0.496005
O	0.909598	0.760818	-1.549155
C	-2.427003	0.210064	-0.476968
Li	1.687524	0.326100	0.175404
H	-3.029125	1.077369	-0.176266
H	-2.466148	0.118929	-1.567690
H	0.499189	-1.843878	1.320937
H	-0.193187	-0.902004	0.264087
H	2.658310	-1.538668	-0.155878
H	3.815927	-0.785907	-0.859485
H	-0.141267	1.360766	0.910908
H	0.689362	1.781163	2.173478
H	-0.009263	0.662988	-1.151563
H	0.946900	1.629182	-1.953823
H	-1.599728	0.263911	2.043314
H	-3.107669	-0.908396	0.949338

O	0.587600	-1.110533	-0.991051
O	1.194219	1.927043	-0.521372
O	0.211658	0.400718	1.778421
O	3.020786	-0.885110	0.099548
Li	1.429002	0.219743	0.342250
H	3.663643	-1.378809	0.610991
H	2.510279	-1.507517	-0.439003
H	-0.536223	0.669123	1.155372
H	-0.137592	-0.314523	2.312848
H	1.648291	2.316419	-1.270833
H	0.248960	1.887532	-0.764765
H	-0.272121	-1.344285	-0.575976
H	0.303336	-0.490050	-1.681889
H	-0.991728	0.997467	-1.662422
O	-1.471354	0.944043	-0.119939
H	-3.016665	0.038384	-1.086205
C	-2.476606	0.057576	-0.130765
H	-3.185994	0.232922	0.688624
O	-1.925652	-1.296231	0.078850
H	-2.599615	-1.950803	-0.124545

Li	-1.375688	0.159649	0.244061
O	-0.390520	1.494630	-0.731314
O	-0.185754	-0.475589	1.635754
O	-3.272115	0.543075	0.487358
O	-1.834524	-1.250049	-1.058894
C	2.769310	-0.147035	-0.267490
O	2.268318	1.122126	0.103077
O	1.834737	-1.171832	-0.061597
H	2.226966	1.182797	1.062799
H	3.648728	-0.388745	0.325931
H	3.029474	-0.069905	-1.320098
H	1.296825	-1.306644	-0.870463
H	-0.452246	-1.111327	2.304629
H	0.576911	-0.862479	1.154402
H	-0.434538	1.311493	-1.681516
H	0.561307	1.493289	-0.516603
H	-1.785895	-2.198410	-0.852686
H	-1.267270	-1.154201	-1.861567
H	-3.691986	1.402861	0.397336
H	-3.558208	0.005636	-0.264483

Table S5. Cartesian Coordinates (Å) for the reactants, products, and intermediates of the $Li(CH_3OH)_4 + CO_2 + 2H_2 \rightarrow Li(CH_3OH)_4 + CH_2(OH)_2$ reaction pathway.

$Li(CH_3OH)_4$			
Li	-0.129803	-0.018199	-0.157710
O	0.757703	0.887076	1.307827
O	-1.811108	0.922064	-0.261251
O	1.144498	-0.099050	-1.608058
O	-0.664291	-1.709513	0.583500
H	0.172737	0.620567	2.051503
C	1.014292	2.286535	1.399257
C	-2.965292	0.661169	-1.053901
H	-2.062689	0.895758	0.688766
C	0.074035	-2.873258	0.938408
H	-1.217623	-1.426361	1.346161
C	2.557517	-0.053177	-1.403559
H	0.947376	-0.259815	-2.532801
H	1.601524	2.567095	0.528485
H	1.581761	2.516433	2.300853
H	0.085405	2.857189	1.400059
H	-2.663409	0.718709	-2.096482
H	-3.736701	1.408516	-0.869526
H	-3.368104	-0.331597	-0.850214
H	0.709630	-3.124833	0.093401
H	-0.595345	-3.709874	1.138462
H	0.697256	-2.693678	1.815400
H	2.710696	0.120245	-0.342963
H	3.006067	0.761672	-1.971259
H	3.023099	-0.997653	-1.684082

CO_2r			
Li	0.914551	0.053528	-0.095252
O	0.015450	-0.885480	-1.497297
O	0.747882	-0.788801	1.677783
O	2.846871	-0.007378	0.106042
O	-0.027305	1.690230	0.093965
H	-0.925699	-0.711573	-1.365376
C	0.198456	-2.163602	-2.090881
C	0.389687	-2.136428	1.981160
H	0.175251	-0.176004	2.200318
C	0.066504	3.026076	-0.389629
H	-0.499129	1.676966	0.961325
C	3.929976	0.873995	-0.162961
H	2.781484	-0.193425	1.052254
H	1.268579	-2.339361	-2.156847
H	-0.225944	-2.191155	-3.094537
H	-0.253681	-2.950318	-1.485853
H	-0.664854	-2.316137	1.769655
H	0.588317	-2.361108	3.028662
H	0.998926	-2.783968	1.355943
H	0.643939	3.650374	0.292953
H	-0.924831	3.460376	-0.519003
H	0.565574	2.991494	-1.354227
H	3.937360	1.055586	-1.233928
H	4.879912	0.422595	0.123155
H	3.806710	1.823939	0.357874
C	-3.390876	0.151016	0.079211
O	-2.732917	-0.526978	-0.600697
O	-4.107238	0.802755	0.701702

eTS1			
Li	-0.798463	0.128865	0.156585
O	-0.133779	-1.107960	1.462364
O	-0.674967	-0.662942	-1.657411
O	-2.711796	0.325482	-0.152629
O	0.367458	1.622378	0.000000
H	0.797059	-1.253982	1.216583
C	-0.657342	-2.242719	2.140729
C	-0.380622	-2.022195	-1.986448
H	-0.037879	-0.067987	-2.148879
C	0.773858	2.830670	0.640397
H	0.725290	1.597965	-0.933212
C	-3.637774	1.396305	0.001207
H	-2.594003	0.109767	-1.095526
H	-1.724093	-2.057068	2.310213
H	-0.161892	-2.383522	3.112717
H	-0.547298	-3.156271	1.537159
H	0.666996	-2.262506	-1.753371
H	-0.572325	-2.214646	-3.051746
H	-1.042532	-2.655566	-1.383674
H	0.386432	3.708705	0.103068
H	1.870855	2.889219	0.692239
H	0.364286	2.820071	1.656837
H	-3.702627	1.614434	1.073274
H	-4.635744	1.109139	-0.361394
H	-3.297771	2.298827	-0.528213
C	2.886698	-0.053346	-0.189907
O	2.347517	-1.056530	0.110656
O	3.554533	0.887639	-0.331943

CO_2p			
Li	0.690489	-0.146816	0.380714
O	0.300454	-0.469809	-1.495040
O	-0.605917	-1.162963	1.335729
O	2.581323	-0.490323	0.620861
O	0.170967	1.711588	0.503186
H	-0.477454	0.128041	-1.579123
C	-0.014856	-1.727420	-2.076160
C	-0.896353	-1.155670	2.721457
H	-1.446272	-0.995446	0.834149
C	0.850540	2.945125	0.365222
H	-0.641082	1.704954	-0.050540
C	3.483118	-0.504689	-0.486828
H	3.026156	-0.788397	1.415922
H	0.809161	-2.406977	-1.869569
H	-0.132344	-1.637294	-3.156790
H	-0.928234	-2.141383	-1.648144
H	0.018007	-1.392917	3.262528
H	-1.646805	-1.908101	2.966236
H	-1.255124	-0.178009	3.048987
H	1.779776	2.878983	0.926825
H	0.257623	3.766736	0.769343
H	1.085839	3.158368	-0.679286
H	2.901875	-0.227288	-1.360470
H	3.900734	-1.500092	-0.636417
H	4.288818	0.214591	-0.341800
C	-2.770660	0.461949	-0.723515
O	-2.798041	-0.529943	-0.007289
O	-1.839147	1.147563	-1.188078

H_2r1			
Li	0.812921	0.292884	-0.228045
O	0.256602	-0.413003	1.494257
O	-0.226550	1.870357	-0.470284
O	2.746674	0.382665	-0.192637
O	0.071712	-1.065864	-1.386401
H	-0.595137	-0.818735	1.215510
C	0.045443	0.345923	2.677042
C	-0.354413	2.685784	-1.620862
H	-1.132564	1.598933	-0.170507
C	0.565496	-2.262367	-1.959365
H	-0.790428	-1.229418	-0.945160
C	3.512806	-0.383349	0.738497
H	3.314818	0.986859	-0.673303
H	0.970017	0.871521	2.905580
H	-0.204842	-0.304457	3.515997
H	-0.750718	1.077858	2.538669
H	0.639203	3.021682	-1.912199
H	-0.966980	3.563118	-1.410514
H	-0.797600	2.135370	-2.452937
H	1.552785	-2.054541	-2.365815
H	-0.079691	-2.604180	-2.769662
H	0.651449	-3.056840	-1.215702
H	2.805047	-0.991227	1.293117
H	4.046450	0.266538	1.431606
H	4.220876	-1.029929	0.220721
C	-2.807969	-0.228229	0.275103
O	-2.622112	0.979611	0.234517
O	-2.034238	-1.206403	0.288430
H	-3.182430	-3.469128	0.507619
H	-3.443907	-4.167538	0.565589

CHTS1			
Li	-0.816423	-0.254993	-0.302459
O	-0.335803	0.101028	1.548787
O	0.392320	-1.617644	-0.844904
O	-2.732466	-0.532399	-0.337673
O	-0.210276	1.403663	-1.094252
H	0.477438	0.627267	1.371210
C	-0.046870	-0.883430	2.531093
C	0.598185	-2.206447	-2.115089
H	1.268034	-1.311679	-0.486149
C	-0.822873	2.652311	-1.355778
H	0.627535	1.532559	-0.596801
C	-3.569752	-0.081593	0.728395
H	-3.243277	-1.041044	-0.969515
H	-0.925931	-1.514900	2.640579
H	0.172702	-0.419479	3.493510
H	0.796596	-1.505678	2.230247
H	0.965676	-1.476812	-2.839536
H	-0.353521	-2.600696	-2.467328
H	1.309892	-3.030425	-2.052340
H	-1.779223	2.460561	-1.837298
H	-0.210876	3.256546	-2.026770
H	-0.998890	3.212991	-0.435690
H	-2.922360	0.432596	1.431661
H	-4.047940	-0.922467	1.230213
H	-4.329160	0.608474	0.361485
C	2.758412	0.505701	0.394621
O	2.684589	-0.671596	0.052128
O	1.863285	1.351426	0.611758
H	3.939704	0.947052	0.566310
H	4.907066	1.315037	0.707385

CHp1			
Li	0.770260	0.081035	0.445659
O	0.557801	-1.264607	-0.959914
O	-0.570504	-0.601051	1.663490

OHTS1			
Li	0.675681	0.064201	0.240472
O	1.077362	-1.210529	-1.162167
O	-0.355193	-0.982020	1.509043

OHp1			
Li	-0.590699	-0.038970	0.102113
O	0.351983	-0.706387	-1.526632
O	-0.577776	-1.021027	1.747312

O	2.684819	0.154516	0.763589
O	0.019942	1.712260	-0.139764
H	-0.426221	-1.205395	-0.992720
C	0.918884	-2.628542	-0.818920
C	-1.225464	0.106133	2.703076
H	-1.226308	-0.826502	0.960301
C	0.503369	2.761591	-0.949852
H	-0.938504	1.523813	-0.369327
C	3.604482	0.048568	-0.322483
H	3.141735	0.418931	1.563738
H	1.998264	-2.680384	-0.689504
H	0.647019	-3.199089	-1.707926
H	0.441103	-3.078604	0.052965
H	-0.484595	0.352548	3.460758
H	-1.999808	-0.508240	3.164672
H	-1.672966	1.030320	2.333762
H	1.550683	2.932270	-0.704193
H	-0.047466	3.686126	-0.767253
H	0.429871	2.515842	-2.011710
H	3.025145	-0.253629	-1.189595
H	4.364581	-0.705136	-0.117499
H	4.082609	1.006460	-0.526894
C	-2.750539	-0.052710	-0.883506
O	-2.066716	-1.053407	-0.518257
O	-2.426763	1.139744	-0.793071
H	-3.738066	-0.276346	-1.321498
H	-3.350877	-3.085972	-0.973533

eTS2

O	2.458152	0.748746	0.664313
O	-0.472781	1.592257	0.043834
H	0.284646	-1.502056	-1.683459
C	1.852924	-2.366552	-0.863429
C	-0.953882	-0.569800	2.727525
H	-1.054164	-1.226563	0.872087
C	-0.270181	2.798652	-0.670608
H	-1.421382	1.339243	-0.010475
C	3.528376	0.854884	-0.274611
H	2.683811	1.204945	1.477019
H	2.613165	-2.079443	-0.140650
H	2.338072	-2.750858	-1.761204
H	1.232982	-3.151236	-0.429947
H	-0.157049	-0.264524	3.401732
H	-1.502296	-1.391412	3.189533
H	-1.630197	0.272649	2.574764
H	0.792133	3.031010	-0.639493
H	-0.821779	3.621706	-0.214307
H	-0.577309	2.700234	-1.712934
H	3.199767	0.347374	-1.175941
H	4.428812	0.371483	0.104023
H	3.742750	1.897945	-0.507367
C	-2.883440	-0.311216	-1.005394
O	-2.055872	-1.242380	-0.634053
O	-2.992683	0.763388	-0.437972
H	-3.470100	-0.539136	-1.902099
H	-1.623562	-1.865477	-1.507576

rFA

O	-0.098473	1.706807	0.756410
O	-2.219022	-0.034780	-0.955722
H	1.199069	-0.217230	-1.599675
C	0.640383	-2.096358	-1.613588
H	-0.023702	-0.508773	2.378539
C	-0.527111	-2.401181	2.081974
H	-1.896488	-0.125417	-1.857304
C	-3.590752	0.330734	-0.917429
H	0.370909	1.621787	1.622637
C	-0.777716	2.954416	0.696222
C	2.765087	0.822051	-0.108805
O	2.344378	-0.114704	0.710434
O	2.671395	0.712446	-1.308857
H	3.200444	1.704916	0.369574
H	2.265828	0.215519	1.656797
H	-0.286943	-2.640570	-1.447430
H	1.366391	-2.391590	-0.855548
H	1.025402	-2.353328	-2.600893
H	-3.866319	0.416915	0.129400
H	-4.214465	-0.431774	-1.384384
H	-3.760263	1.289726	-1.408100
H	-1.142999	-2.934785	1.362573
H	-0.925219	-2.572965	3.081967
H	0.493600	-2.782610	2.032613
H	-1.274944	3.009217	-0.268550
H	-0.075157	3.783683	0.778604
H	-1.522284	3.037384	1.489048

H_2r2

Li	-0.895760	0.098551	-0.278038
O	0.288248	-0.537125	-1.656053
O	-0.567749	1.988921	-0.361584
O	-2.725355	-0.484565	-0.563543
O	-0.396534	-0.597144	1.440275
H	0.978826	0.153161	-1.731443
C	0.884455	-1.822428	-1.821885
C	-1.309839	3.141497	-0.736781
H	0.379750	2.106495	-0.608443
C	-0.744460	0.032488	2.661093
H	0.587498	-0.674308	1.386015
C	-3.279524	-1.637585	0.070185
H	-3.157567	-0.329930	-1.406028
H	0.099824	-2.561633	-1.680103
H	1.668981	-1.984958	-1.084501
H	1.291606	-1.930867	-2.827017
H	-2.344810	2.970039	-0.452372
H	-1.256751	3.313095	-1.812722
H	-0.942997	4.026490	-0.216460
H	-1.830512	0.068388	2.726607
H	-0.362437	1.054029	2.705872
H	-0.363061	-0.530753	3.513697
H	-2.660762	-1.840891	0.938412
H	-3.251603	-2.501814	-0.593215
H	-4.305438	-1.450784	0.386902
C	2.800227	0.256826	0.550060
O	3.861866	0.055624	-0.250864
O	2.203288	-0.700497	1.023429
H	2.625673	1.289252	0.842857
H	4.115795	0.902826	-0.643261

CHTS2

Li	0.807766	0.261950	-0.276627
O	0.428031	-0.674125	1.387742
O	-0.198393	1.885522	-0.104599
O	2.747269	0.257534	-0.408626
O	-0.147358	-0.678647	-1.646712
H	-0.496405	-0.988027	1.259557
C	0.490083	0.053959	2.604644
C	-0.216926	3.152106	-0.724009
H	-1.091940	1.431156	-0.211234
C	-0.198110	-2.036530	-2.027899
H	-1.052565	-0.371420	-1.345132
C	3.535074	-0.780997	0.172055
H	3.242094	0.704926	-1.097335
H	1.509061	0.416086	2.726929
H	0.244518	-0.584051	3.455450
H	-0.183193	0.911383	2.585590
H	0.771568	3.599154	-0.625967
H	-0.940754	3.814544	-0.245028
H	-0.463121	3.078363	-1.786172
H	0.817943	-2.378772	-2.219383
H	-0.781729	-2.167086	-2.941770
H	-0.634814	-2.655740	-1.241152
H	2.896501	-1.285889	0.890185
H	4.404601	-0.369076	0.684308
H	3.858906	-1.497453	-0.583017
C	-2.867615	-0.207509	0.404156
O	-2.151873	-1.345853	0.946084
O	-2.223355	0.388751	-0.541861
H	-3.923185	-0.464401	0.251620
H	-2.690390	-1.731174	1.642534

CHp2

Li	-0.860019	0.317933	0.279430
O	-0.679731	-0.822476	-1.287412
O	0.190183	1.857152	-0.172368
O	-2.774724	0.420726	0.591083
O	0.194997	-0.511167	1.647319
H	0.238816	-1.166925	-1.208026
C	-0.831854	-0.240424	-2.573322
C	0.311537	3.182607	0.295008
H	1.072799	1.379535	-0.095787
C	0.229360	-1.815720	2.185726
H	1.078029	-0.286416	1.233107
C	-3.653243	-0.640296	0.217957
H	-3.186257	0.974130	1.257216
H	-1.839791	0.164247	-2.640601
H	-0.705119	-0.987635	-3.358623
H	-0.120609	0.571910	-2.724708
H	-0.661498	3.665809	0.217550
H	1.023798	3.748951	-0.308018
H	0.635903	3.214614	1.337972
H	-0.776106	-2.080479	2.509487
H	0.893301	-1.866472	3.051184
H	0.562986	-2.544439	1.443808
H	-3.105706	-1.259306	-0.485823
H	-4.551219	-0.250849	-0.261603
H	-3.930660	-1.242913	1.082865
C	2.709248	-0.397299	-0.698248
O	1.907511	-1.563106	-1.005825
O	2.204990	0.327195	0.244960
H	3.771070	-0.669087	-0.651736
H	2.354332	-2.056303	-1.699191
H	4.757652	0.795988	2.083608
H	4.132240	0.742036	1.674259

OHTS2

Li	1.081078	-0.116698	0.633265
C	-2.483815	0.513790	-1.274101
H	-2.652068	-0.320989	-2.217843
H	-2.815218	-1.066059	-2.914377
H	-1.854359	-0.803038	2.284527
H	-2.164493	0.885988	2.783057
O	1.242728	1.389637	-0.693712
O	0.204733	-1.525385	-0.573209

Li	-0.811592	-0.153122	0.374065
O	-0.470410	1.459147	-0.626869
O	0.444898	-0.152252	1.848145
O	-2.730210	-0.169101	0.702974
O	-0.134100	-1.564869	-0.750471
H	0.387188	1.100304	-1.040916
C	-0.254639	2.763241	-0.133719
C	0.726207	-1.330043	2.582540

Li	-0.817460	-0.142964	0.480597
O	-0.429633	1.375893	-0.648447
O	0.549716	-0.053322	1.843786
O	-2.721280	-0.048958	0.848923
O	-0.311461	-1.578862	-0.704136
H	0.388109	1.013371	-1.084637
C	-0.266956	2.761918	-0.401687
C	0.961213	-1.117507	2.689274

O	2.771821	-1.148692	0.340128	H	1.271059	0.152749	1.409373	H	1.346914	0.298215	1.373130
O	-0.466966	0.613616	1.592880	C	-0.737153	-2.241019	-1.828884	C	-1.006507	-2.431991	-1.594655
O	-3.248914	0.005910	-0.177843	H	0.646578	-0.985147	-1.088079	H	0.463821	-1.145028	-1.170570
O	-1.197182	0.582828	-0.931907	C	-3.605866	0.577315	-0.142748	C	-3.585765	0.596868	-0.091680
H	-2.925872	1.458681	-1.663352	H	-3.235573	-0.724975	1.297915	H	-3.229666	-0.362068	1.606403
H	-4.173483	-0.045866	-0.469648	H	-1.120466	3.062525	0.456512	H	-1.216916	3.152378	-0.013919
C	1.372238	2.737052	-0.229248	H	-0.131848	3.478983	-0.950312	H	-0.011824	3.297397	-1.327711
H	0.316019	1.295624	-1.040456	H	0.629841	2.806797	0.505915	H	0.517098	2.951492	0.350264
C	-1.375206	0.141457	2.590491	H	-0.164712	-1.593640	3.149564	H	1.788807	-0.804159	3.342824
H	-0.968278	0.683989	0.728181	H	1.543266	-1.168240	3.287689	H	1.273914	-1.997794	2.104968
C	3.899205	-0.528701	-0.299906	H	0.980541	-2.160142	1.920570	H	0.108650	-1.399053	3.320528
H	2.267094	-1.629761	-0.341941	H	-1.654528	-2.714680	-1.479172	H	-1.913963	-2.787510	-1.089258
H	-0.396722	-0.780778	-0.905916	H	-0.082396	-3.020717	-2.226163	H	-0.394686	-3.306380	-1.866770
C	-0.684890	-2.574537	-0.168369	H	-0.989138	-1.557004	-2.643653	H	-1.298551	-1.903476	-2.516054
H	-0.194717	-3.169975	0.617138	H	-2.969464	1.170605	-0.791657	H	-2.941204	0.968865	-0.895472
H	-0.921470	-3.233482	-1.020104	H	-4.243591	1.238059	0.444595	H	-4.108419	1.444475	0.374593
H	-1.624690	-2.152196	0.225658	H	-4.222646	-0.085999	-0.749265	H	-4.316754	-0.112788	-0.505241
H	2.380104	2.848212	0.197306	C	2.753226	0.278792	-0.928686	C	2.755417	-0.201537	-0.755538
H	0.625783	2.962902	0.551431	O	2.641360	0.655429	0.503147	O	2.716657	0.661400	0.403141
H	1.262937	3.452943	-1.060533	O	1.538353	0.159300	-1.452713	O	1.635953	-0.061823	-1.541689
H	4.453563	0.004625	0.483721	H	3.518480	0.814086	0.863057	H	2.879242	1.563854	0.088112
H	3.569828	0.189162	-1.068097	H	1.982907	-3.162134	-0.226570	H	3.663700	0.043263	-1.334915
H	4.560866	-1.287042	-0.747489	H	3.350815	1.077310	-1.395313	H	2.833935	-1.217130	-0.340180
H	-0.803001	-0.020524	3.515058	H	3.328683	-0.660318	-0.951002	H	1.956145	0.729823	-2.544794

OHp2

Li	-0.796320	-0.183608	0.237194
O	-0.169080	1.534167	-0.396220
O	0.398326	-0.508766	1.717296
O	-2.680273	0.154701	0.614244
O	-0.619679	-1.561918	-1.064100
H	0.689580	1.356526	-0.839223
C	-0.025749	2.654644	0.462029
C	0.369656	-1.573087	2.655859
H	1.282776	-0.478768	1.293157
C	-1.531967	-2.067572	-2.030520
H	0.297880	-1.828051	-1.317421
C	-3.457310	1.061594	-0.168471
H	-3.250396	-0.362868	1.185696
H	-0.993279	2.852835	0.918124
H	0.284619	3.537805	-0.097503
H	0.694199	2.458450	1.258359
H	-0.606237	-1.567329	3.136650
H	1.133673	-1.437520	3.422011
H	0.518338	-2.537714	2.167745
H	-2.527336	-1.734759	-1.746689
H	-1.512342	-3.157407	-2.049369
H	-1.297417	-1.690071	-3.026286
H	-2.758194	1.601515	-0.799323
H	-3.989831	1.767654	0.468475
H	-4.168654	0.526810	-0.797728
C	3.215672	0.357069	-0.592912
O	2.720316	-0.603846	0.303803
O	2.221646	0.839593	-1.468323
H	2.573972	-1.432655	-0.210974
H	3.568206	1.200882	-0.008416
H	4.032089	-0.072150	-1.174203
H	2.025456	0.120309	-2.104180

Table S6. Cartesian Coordinates (Å) for the reactants, products, and intermediates of the $Li(NH_3)_4$ + 2 C_2H_4 → $Li(NH_3)_4$ + $C_5H_8O_2$ reaction pathway.

$Li(NH_3)_4$			
Li	0.000009	-0.000012	-0.000099
N	-0.002118	-2.055733	0.121696
N	1.790986	0.638982	-0.790750
N	-1.545383	0.617417	-1.213109
N	-0.243470	0.799328	1.882126
H	0.115071	-2.493213	-0.788954
H	-0.871010	-2.415284	0.509192
H	0.748278	-2.405079	0.712681
H	1.834706	1.651999	-0.870016
H	1.953092	0.265471	-1.722743
H	2.583914	0.355820	-0.220235
H	-0.249736	1.816274	1.868390
H	0.501427	0.520031	2.515792
H	-1.117792	0.507308	2.311889
H	-1.581365	1.629988	-1.301480
H	-2.451702	0.322489	-0.858137
H	-1.465022	0.244279	-2.155821

CO_2r			
Li	1.333803	-0.001072	-0.011985
N	3.288410	-0.001790	-0.674313
N	1.437284	0.005041	2.045205
N	0.482066	1.749026	-0.700506
N	0.480236	-1.753232	-0.692624
H	3.794477	0.814733	-0.336390
H	3.384422	-0.003755	-1.687587
H	3.796385	-0.815695	-0.333014
H	0.551863	0.006969	2.544983
H	1.954490	0.821459	2.364792
H	1.954513	-0.808861	2.371057
H	-0.473211	-1.960927	-0.410612
H	1.060038	-2.514123	-0.346333
H	0.506496	-1.809757	-1.707407
H	-0.469668	1.962219	-0.416791
H	0.505285	1.799153	-1.715720
H	1.065788	2.509953	-0.360850
C	-2.796321	0.000405	0.011418
O	-2.791412	-1.156081	0.010163
O	-2.792379	1.156845	0.009460

eTS			
Li	1.293410	0.027261	-0.000221
N	3.364924	0.057270	0.000105
N	0.564372	1.955620	-0.000046
N	0.579950	-0.990143	-1.651582
N	0.580585	-0.990700	1.651083
H	3.735682	0.535128	-0.815264
H	3.760648	-0.877679	-0.000233
H	3.735234	0.534370	0.816127
H	-0.454999	1.930284	0.000547
H	0.838609	2.497130	-0.815237
H	0.839599	2.497302	0.814699
H	-0.345116	-1.335355	1.401755
H	0.460091	-0.408329	2.475111
H	1.125227	-1.798050	1.940656
H	-0.345463	-1.335404	-1.401911
H	1.124772	-1.797069	-1.942017
H	0.458722	-0.407278	-2.475156
C	-2.596192	-0.028498	0.000152
O	-2.564809	1.141235	0.000533
O	-2.293302	-1.162507	-0.000065

CO_2p			
Li	1.240280	0.024100	-0.012381
N	3.327989	-0.051503	0.129458
N	0.524386	1.895792	-0.446936
N	0.482236	-1.267950	-1.436119
N	0.296483	-0.532660	1.737640
H	3.774493	0.282797	-0.715506
H	3.662654	-0.992932	0.293162
H	3.663174	0.522382	0.893309
H	-0.478068	1.688418	-0.308671
H	0.621815	2.252097	-1.389903
H	0.749636	2.665629	0.171388
H	0.042075	0.242095	2.338621
H	0.606590	-1.282158	2.343150
H	-0.575619	-0.841504	1.288861
H	-0.468493	-1.307819	-1.044210
H	0.810002	-2.223023	-1.510355
H	0.396902	-0.918855	-2.382807
C	-2.577155	-0.045518	-0.027190
O	-2.184932	1.116914	-0.004583
O	-2.000159	-1.140923	0.046451

EtR			
Li	-1.638042	-0.632565	0.030622
N	-2.920585	-2.279927	-0.124769
N	-2.586895	1.185970	-0.215503
N	-0.637620	-0.554322	1.819304
N	-0.162584	-0.645692	-1.408071
H	-3.570804	-2.341792	0.648780
H	-2.386441	-3.140056	-0.138043
H	-3.468376	-2.254966	-0.975876
H	-1.734267	1.718304	-0.434434
H	-3.000133	1.612285	0.604702
H	-3.234436	1.341745	-0.978072
H	0.004700	0.366531	-1.394725
H	-0.313880	-0.913029	-2.372431
H	0.705911	-1.079707	-1.114690
H	0.004511	0.220974	1.592941
H	-0.056731	-1.347401	2.063156
H	-1.130655	-0.290961	2.663672
C	0.852022	2.309212	0.040903
O	0.024932	2.252176	-0.878218
O	1.111516	1.570103	0.988942
C	3.126610	-1.134872	0.500765
C	3.500527	-1.412038	-0.736156
H	3.251686	-1.861203	1.294529
H	2.693693	-0.177819	0.766010
H	3.939947	-2.364769	-1.002016
H	3.396654	-0.684687	-1.530962

EtTS1			
Li	-1.801591	-0.225350	0.011996
N	-3.792823	-0.878073	-0.019223
N	-0.898483	-0.576187	1.837109
N	-0.662830	-1.146725	-1.455483
N	-1.637400	1.807039	-0.323592
H	-4.352439	-0.377374	0.660003
H	-3.872180	-1.864456	0.195054
H	-4.221946	-0.732610	-0.924687
H	-0.120602	0.086327	1.737097
H	-0.482783	-1.489313	1.974460
H	-1.377735	-0.344351	2.698123
H	-1.482191	2.313540	0.540540
H	-2.265566	2.364580	-0.888319
H	-0.721177	1.799087	-0.786273
H	0.036190	-0.408929	-1.583098
H	-1.044523	-1.363195	-2.367560
H	-0.145201	-1.963581	-1.153373
C	1.531376	1.035946	-0.039399
O	1.138164	1.337458	1.080161
O	1.089348	1.183781	-1.179679
C	2.694606	-1.755938	0.040136
C	3.195828	-0.496963	0.036231
H	2.508717	-2.291896	-0.881102
H	2.426999	-2.254557	0.962272
H	3.592190	-0.072642	-0.874827
H	3.516822	-0.035129	0.958367

EtP			
Li	-2.171253	0.080239	0.000428
N	-4.265261	0.116375	0.004357
N	-1.363665	-0.911543	-1.615275
N	-1.315108	1.935959	-0.011477
N	-1.358096	-0.893828	1.623935
H	-4.627122	0.593708	-0.811772
H	-4.623557	0.598531	0.819225
H	-4.660509	-0.815598	0.007984
H	-0.458303	-1.074677	-1.144902
H	-1.173125	-0.352415	-2.437499
H	-1.695422	-1.808672	-1.946106
H	-0.454727	-1.062974	1.151914
H	-1.689033	-1.786759	1.966715
H	-1.163767	-0.325096	2.438657
H	-0.328765	1.613606	-0.009437

EtR2			
Li	-1.967389	-1.197103	-0.016114
N	-4.025130	-1.570497	0.062584
N	-1.165807	-0.599871	1.785709
N	-0.824350	-2.792369	-0.590654
N	-1.473828	0.348664	-1.282396
H	-4.279075	-2.140901	0.859411
H	-4.354331	-2.047646	-0.767339
H	-4.541925	-0.702974	0.135732
H	-0.353157	-0.138371	1.349370
H	-0.800054	-1.334825	2.378234
H	-1.605260	0.076971	2.396406
H	-0.535063	0.472838	-0.875104
H	-1.928477	1.251610	-1.219456
H	-1.355737	0.147506	-2.267256
H	0.097331	-2.343273	-0.439791

EtTS2			
Li	-2.903530	-0.361981	-0.009267
N	-4.891729	-1.003242	0.133044
N	-1.862250	-0.514910	1.761880
N	-1.791517	-1.403919	-1.372127
N	-2.701222	1.626023	-0.515082
H	-5.350920	-1.005971	-0.769190
H	-5.436908	-0.410199	0.746204
H	-4.944731	-1.945010	0.500803
H	-1.151523	0.177601	1.478083
H	-1.374100	-1.388721	1.914579
H	-2.224538	-0.223958	2.660954
H	-1.733139	1.688678	-0.160908
H	-3.230818	2.362719	-0.066377
H	-2.674237	1.850346	-1.501870
H	-0.883082	-0.944931	-1.173445

H	-1.428362	2.539224	0.793902
H	-1.428672	2.528194	-0.824961
C	1.718716	-0.219649	-0.001699
O	0.971566	-1.239312	0.001868
O	1.329990	0.963756	-0.004745
C	3.220468	-0.508033	-0.003686
C	4.104826	0.674794	0.006990
H	3.415619	-1.166427	0.850763
H	3.414492	-1.149121	-0.871923
H	5.178654	0.557734	0.014987
H	3.674771	1.663053	0.003780

EtP2

H	-0.850510	-3.094064	-1.556868
H	-0.834715	-3.636199	-0.031031
C	1.848130	-0.265387	0.055745
O	0.955290	0.611624	0.244046
O	1.638745	-1.477316	-0.134364
C	3.288154	0.247432	0.077177
C	4.336404	-0.766737	-0.155546
H	3.344546	1.061407	-0.654883
H	3.425729	0.755566	1.039187
H	5.379127	-0.485176	-0.168680
H	4.058705	-1.796830	-0.308287
C	-1.089806	4.144477	-0.573748
C	-0.677621	3.537582	0.525297
H	0.035755	2.722216	0.499110
H	-1.042253	3.846560	1.497315
H	-0.720522	3.854196	-1.549038
H	-1.797976	4.962542	-0.546401

LacTS

H	-1.975614	-1.276971	-2.359762
H	-1.652080	-2.397895	-1.237524
C	0.801995	0.900096	-0.033628
O	-0.096380	1.462270	0.652371
O	0.643645	-0.110973	-0.747299
C	2.185662	1.548830	0.030924
C	3.284041	0.817957	-0.653858
H	2.063400	2.551900	-0.398104
H	2.413648	1.732211	1.083106
H	4.281037	1.231882	-0.587709
H	3.043081	0.310233	-1.575396
C	4.673141	-1.755673	0.156032
C	3.610934	-1.041743	0.587885
H	4.577535	-2.482071	-0.639247
H	5.669123	-1.579370	0.538629
H	2.605961	-1.305679	0.292604
H	3.702758	-0.413690	1.463661

LacP

Li	-3.163881	0.208112	-0.007366
N	-5.246535	0.433582	-0.003845
N	-2.451652	-0.871644	-1.611114
N	-2.138771	1.975102	-0.034236
N	-2.443690	-0.820044	1.626475
H	-5.562401	0.969068	-0.802794
H	-5.562907	0.917026	0.827445
H	-5.722704	-0.459305	-0.032466
H	-1.563678	-1.109188	-1.138762
H	-2.213728	-0.342876	-2.441010
H	-2.863141	-1.739781	-1.929513
H	-1.560725	-1.076630	1.154698
H	-2.854187	-1.674524	1.980954
H	-2.195468	-0.261320	2.433436
H	-1.186215	1.562713	-0.014943
H	-2.204992	2.597986	0.761410
H	-2.187305	2.563607	-0.856865
C	0.684021	-0.449035	0.014379
O	-0.157095	-1.393259	0.009035
O	0.404987	0.766947	0.020757
C	2.151127	-0.865237	0.018001
C	3.152718	0.273267	-0.024064
H	2.303159	-1.482261	0.907042
H	2.293721	-1.541778	-0.827610
C	4.598009	-0.210810	-0.001100
H	2.976746	0.941499	0.819873
H	2.981748	0.875519	-0.916955
H	4.749722	-0.836803	0.891276
C	5.598638	0.882059	-0.018265
H	4.776985	-0.889375	-0.842999
H	5.317920	1.892932	0.240527
H	6.643418	0.679216	-0.203646

C_2H_4

Li	-2.657598	-0.095727	-0.043276
N	-4.713938	-0.513885	-0.025112
N	-2.262984	1.906688	-0.306046
N	-1.729663	-0.579156	1.724481
N	-1.628198	-1.138971	-1.488639
H	-5.176296	0.121991	0.612699
H	-4.907470	-1.454523	0.294829
H	-5.153161	-0.404211	-0.930439
H	-1.286974	1.787472	0.026985
H	-2.688975	2.624017	0.267051
H	-2.216691	2.280386	-1.245587
H	-0.657623	-0.960012	-1.190454
H	-1.702405	-0.803013	-2.441214
H	-1.741739	-2.144385	-1.532260
H	-0.896150	-0.019421	1.454953
H	-1.419752	-1.533112	1.860504
H	-2.037945	-0.244454	2.628593
C	1.099190	0.726684	-0.145630
O	1.056820	-0.507752	-0.623311
O	0.229210	1.150072	0.700284
C	2.462616	1.384336	-0.206784
C	3.555340	0.336745	-0.403815
H	2.504792	2.147759	-0.988764
H	2.615320	1.908035	0.741049
H	4.535281	0.780842	-0.224232
H	3.550015	-0.023545	-1.433777
C	2.115121	-1.643456	0.178057
C	3.341558	-0.849061	0.544360
H	1.538234	-2.040529	1.004681
H	2.254499	-2.364783	-0.617999
H	3.250524	-0.467150	1.563635
H	4.221599	-1.496961	0.533873

δ-lactone

C	-0.000000	-0.000000	0.659538
C	0.000000	-0.000000	-0.659538
H	0.000000	0.920763	1.227183
H	-0.000000	-0.920763	1.227183
H	0.000000	0.920763	-1.227183
H	-0.000000	-0.920763	-1.227183

C	-1.719179	-0.061151	0.324971
C	-0.960800	-1.266976	-0.174499
C	-1.117156	1.190316	-0.287626
H	-1.663922	-0.012132	1.414570
H	-2.769711	-0.175425	0.057485
C	0.349863	1.276046	0.106030
H	-1.643945	2.086779	0.036164
H	-1.212701	1.143328	-1.374682
H	0.436216	1.582227	1.151411
H	0.899447	2.014301	-0.472297
C	1.129571	-0.017063	0.013435
O	0.455987	-1.183926	0.035733
O	2.325566	-0.039155	-0.009721
H	-1.125559	-1.402069	-1.245790
H	-1.266043	-2.179396	0.331168

Table S7. Cartesian Coordinates (Å) for the reactants, products, and intermediates of the $Li(NH_2CH_3)_4 + 2\ C_2H_4 \rightarrow Li(NH_2CH_3)_4 + C_5H_8O_2$ reaction pathway.

$Li(NH_2CH_3)_4$			
Li	0.000082	-0.268028	0.000075
N	0.473285	0.826367	-1.696485
N	-1.534619	-1.571332	-0.470398
N	1.534997	-1.571240	0.470062
N	-0.473227	0.826124	1.696735
H	0.870764	0.096000	-2.281813
C	1.399822	1.961430	-1.613232
H	-0.380889	1.109458	-2.164231
H	-1.570252	-2.216047	0.318669
H	-1.163893	-2.128468	-1.240050
C	-2.897571	-1.130976	-0.799337
H	-0.869989	0.095624	2.282375
C	-1.400586	1.960522	1.613526
H	0.380919	1.109936	2.164089
H	1.164457	-2.128868	1.239442
C	2.897844	-1.130677	0.799162
H	1.570768	-2.215538	-0.319346
H	3.316193	-0.583836	-0.043693
H	3.572144	-1.955380	1.038050
H	2.867840	-0.457957	1.654559
H	-2.321342	1.638645	1.131797
H	-0.961957	2.743510	0.998181
H	-1.654855	2.389291	2.584846
H	2.320650	1.640307	-1.131135
H	0.960449	2.744255	-0.998209
H	1.654108	2.390156	-2.584567
H	-2.867710	-0.457764	-1.654352
H	-3.316131	-0.584732	0.043800
H	-3.571618	-1.955737	-1.038734

CO_2r			
Li	0.973686	0.322844	-0.144200
N	3.041809	0.168478	-0.300889
N	0.483721	2.275193	-0.612299
N	0.079025	-0.769937	-1.654755
N	0.150713	-0.204753	1.684549
H	3.175022	0.554453	-1.232176
C	3.698218	-1.140592	-0.206574
H	3.484952	0.825363	0.331726
H	-0.534400	2.276009	-0.683623
H	0.801598	2.398181	-1.573344
C	0.913869	3.427587	0.192608
H	0.174980	0.604235	2.294599
C	0.644198	-1.386807	2.398674
H	-0.825264	-0.331033	1.436746
H	-0.823572	-0.310454	-1.775108
C	-0.122598	-2.221481	-1.557709
H	0.590243	-0.548887	-2.507080
H	0.837572	-2.717392	-1.427273
H	-0.611642	-2.650362	-2.434475
H	-0.737069	-2.441830	-0.687306
H	1.680247	-1.228429	2.691919
H	0.616111	-2.247990	1.734138
H	0.068972	-1.628822	3.294633
H	3.243677	-1.820988	-0.923606
H	3.543983	-1.554168	0.787922
H	4.771580	-1.106968	-0.402958
H	2.001054	3.456114	0.238753
H	0.537648	3.323476	1.208783
H	0.564294	4.383285	-0.202861
C	-3.747846	-0.107119	0.058848
O	-4.671809	0.471276	-0.315985
O	-2.838561	-0.710615	0.457468

eTS			
Li	-0.864777	0.029861	-0.317926
N	-2.870011	-0.361435	-0.734746
N	0.302801	-0.935460	-1.726170
N	-0.441325	2.024854	-0.636887
N	-0.296077	-0.520777	1.596329
H	-2.999557	0.128792	-1.613619
C	-3.880216	0.071031	0.236786
H	-2.987621	-1.345081	-0.947374
H	1.166730	-0.392928	-1.678725
H	-0.070049	-0.736981	-2.650672
C	0.624570	-2.364552	-1.619096
H	0.713167	-0.491648	1.487282
C	-0.704193	-1.822000	2.134398
H	-0.520906	0.212683	2.257897
H	0.575898	2.040711	-0.526198
C	-1.031474	3.119202	0.145915
H	-0.582405	2.204813	-1.629099
H	-2.109336	3.138806	-0.004551
H	-0.632215	4.100844	-0.116054
H	-0.843458	2.951338	1.204936
H	-0.439292	-2.604339	1.426316
H	-1.785151	-1.844308	2.262351
H	-0.242242	-2.062996	3.093932
H	-3.749318	1.130969	0.443353
H	-3.736313	-0.467094	1.171432
H	-4.907461	-0.089066	-0.096501
H	-0.291727	-2.952538	-1.641495
H	1.123592	-2.547954	-0.670291
H	1.278961	-2.720866	-2.416951
C	3.441710	0.346637	0.258747
O	4.323045	1.064883	0.041887
O	2.684822	-0.476749	0.604065

CO_2p			
Li	-0.692997	-0.038287	-0.419278
N	-2.678725	-0.377240	-0.999102
N	0.635473	-1.081770	-1.624801
N	-0.111465	1.946988	-0.619810
N	-0.473846	-0.539851	1.562422
H	-2.791027	-0.204123	-1.989827
C	-3.636399	0.422413	-0.229887
H	-2.854624	-1.364625	-0.861785
H	1.404227	-0.416706	-1.490327
H	0.424298	-1.078756	-2.614903
C	1.093786	-2.415869	-1.222607
H	0.548043	-0.429565	1.539090
C	-0.830291	-1.859701	2.083040
H	-0.813576	0.175555	2.192915
H	0.878394	1.729746	-0.777308
C	-0.219437	2.831767	0.543658
H	-0.435423	2.431049	-1.447615
H	-1.265684	2.993645	0.803419
H	0.249882	3.806408	0.393364
H	0.272038	2.359860	1.391902
H	-0.435853	-2.628252	1.421275
H	-1.914338	-1.974288	2.113427
H	-0.442071	-2.053890	3.085559
H	-3.430698	1.478592	-0.390268
H	-3.500540	0.218896	0.830082
H	-4.680282	0.231079	-0.487139
H	0.267574	-3.126416	-1.251799
H	1.467948	-2.362160	-0.202968
H	1.898867	-2.803588	-1.850694
C	2.931765	0.521257	0.344440
O	2.607660	0.914906	-0.784532

EtR			
Li	-1.340662	-0.159803	0.166175
N	-2.906704	-1.527459	-0.085988
N	-1.909231	1.784574	-0.292146
N	-0.659771	-0.012280	2.121876
N	0.218685	-0.729667	-1.041879
H	-3.747986	-1.211343	0.379108
C	-2.547130	-2.873782	0.369287
H	-3.116081	-1.536016	-1.076405
H	-1.172952	2.213261	0.278692
H	-2.790473	2.081436	0.108143
C	-1.796415	2.290437	-1.664017
H	0.730837	0.155985	-0.949494
C	-0.008089	-1.039367	-2.453110
H	0.835599	-1.426072	-0.641143
H	-0.249417	0.918080	1.994776
C	0.374192	-0.936319	2.595940
H	-1.375127	0.089494	2.830896
H	-0.029950	-1.944735	2.681489
H	0.798088	-0.655164	3.562522
H	1.187553	-0.963559	1.874059
H	-0.635322	-0.269814	-2.899637
H	-0.531093	-1.991225	-2.552212
H	0.911074	-1.099567	-3.041146
H	-2.334840	-2.845690	1.435815
H	-1.638257	-3.190945	-0.137455
H	-3.321798	-3.622480	0.191087
H	-2.497001	1.772411	-2.319104
H	-0.786826	2.104675	-2.023120
H	-1.983452	3.363416	-1.745898
C	1.405179	2.431081	0.525058
O	0.433069	2.570035	1.278058

EtTS1			
Li	-1.498377	0.248458	-0.300751
N	-3.532073	-0.082829	-0.705407
N	-0.323933	-1.086164	-1.383257
N	-0.835508	2.123000	-0.905700
N	-1.132493	0.167690	1.725909
H	-4.062090	0.498290	-0.068309
C	-3.913311	-1.489911	-0.545264
H	-3.760411	0.238581	-1.637540
H	0.468229	-0.449538	-1.501417
H	-0.658509	-1.302896	-2.313893
C	0.160162	-2.311856	-0.736683
H	-0.124089	0.326490	1.607779
C	-1.362515	-1.002766	2.574096
H	-1.484681	0.994584	2.192164
H	0.129972	1.822634	-1.082094
C	-0.818238	3.214446	0.072968
H	-1.196849	2.462669	-1.788169
H	-1.833393	3.470263	0.377338
H	-0.335848	4.121583	-0.297767
H	-0.267190	2.887045	0.951941
H	-0.975042	-1.891011	2.079475
H	-2.430972	-1.151097	2.731119
H	-0.883664	-0.931721	3.553322
H	-3.664244	-1.815769	0.462163
H	-3.335564	-2.098026	-1.237747
H	-4.974121	-1.682403	-0.718381
H	-0.675535	-2.971326	-0.502693
H	0.656638	-2.045605	0.193385
H	0.877116	-2.866716	-1.344650
C	2.196314	0.687483	0.035791
O	1.810305	0.904630	-1.117179

O	2.341745	-0.102867	1.223108

EtP

O	1.614380	1.733947	-0.466182
C	3.817714	-0.882728	0.076750
C	3.882396	-1.833978	-0.838015
H	3.366565	0.080993	-0.125553
H	4.222525	-1.036959	1.069074
H	3.495041	-1.682302	-1.837449
H	4.337742	-2.794561	-0.634969

EtR2

O	1.637667	0.655957	1.126846
C	4.287526	-0.161524	0.097194
C	4.260641	-1.492974	-0.143964
H	4.369581	0.207886	1.109141
H	4.558290	0.528094	-0.689313
H	4.114424	-2.207353	0.654590
H	4.303864	-1.884008	-1.151164

EtTS2

Li	-1.478215	0.001731	-0.377227
N	-3.550765	-0.247832	-0.559059
N	-0.417767	-1.078803	-1.788651
N	-0.799958	1.937194	-0.680852
N	-0.896566	-0.541142	1.512466
H	-3.855504	-0.057143	-1.504882
C	-4.300072	0.573168	0.395841
H	-3.729121	-1.230633	-0.395102
H	0.404262	-0.467701	-1.695621
H	-0.735508	-0.995203	-2.746034
C	-0.010844	-2.461208	-1.521761
H	0.107767	-0.520814	1.273126
C	-1.249556	-1.835689	2.093558
H	-1.031881	0.185345	2.204207
H	0.157933	1.614791	-0.878826
C	-0.770644	2.897073	0.423280
H	-1.124722	2.397602	-1.521752
H	-1.782220	3.197815	0.696766
H	-0.195925	3.799734	0.201994
H	-0.316274	2.426154	1.292881
H	-1.081435	-2.620588	1.358407
H	-2.306464	-1.857237	2.363009
H	-0.669698	-2.088389	2.984661
H	-4.096870	1.623929	0.200627
H	-3.952832	0.353949	1.403199
H	-5.380625	0.418144	0.361163
H	-0.881638	-3.116351	-1.480507
H	0.493178	-2.494152	-0.558765
H	0.678694	-2.861499	-2.269082
C	2.355894	0.217141	-0.187810
O	1.751711	0.730599	-1.170596
O	1.823874	-0.440291	0.729020
C	3.871300	0.424208	-0.167439
C	4.572355	-0.056210	1.040448
H	4.055243	1.487965	-0.348120
H	4.256217	-0.062623	-1.073356
H	5.627914	0.130624	1.173597
H	4.034271	-0.628191	1.778669

EtP2

Li	1.788308	-0.540478	0.187623
N	3.863447	-0.411852	-0.062653
N	1.039128	-2.445915	-0.133449
N	1.090904	-0.110664	2.090632
N	0.881599	0.769502	-1.097393
H	4.348817	-1.113068	0.481863
C	4.373971	0.925318	0.253022
H	4.038107	-0.634714	-1.034515
H	0.182937	-2.241709	0.397695
H	1.514106	-3.193108	0.357109
C	0.664834	-2.897471	-1.476270
H	-0.062050	0.381583	-0.946187
C	1.197193	0.783153	-2.525071
H	0.826667	1.723646	-0.762107
H	0.184083	-0.560154	1.903381
C	0.876992	1.276067	2.506293
H	1.511387	-0.630971	2.850306
H	1.831268	1.777170	2.668842
H	0.284007	1.371431	3.419359
H	0.353468	1.810204	1.715957
H	1.220892	-0.237230	-2.903778
H	2.182648	1.219896	-2.693025
H	0.476002	1.342703	-3.126165
H	4.183524	1.142346	1.301832
H	3.832791	1.661612	-0.337142
H	5.442617	1.047188	0.063579
H	1.549449	-3.006552	-2.104307
H	0.014021	-2.151711	-1.926816
H	0.127390	-3.848858	-1.479565
C	-2.071884	-0.956715	0.440656
O	-1.295787	-1.494485	1.276926
O	-1.719537	-0.268480	-0.540013
C	-3.565069	-1.171285	0.692430
C	-4.467017	-0.798236	-0.416133
H	-3.799067	-0.599998	1.601853
H	-3.701556	-2.212706	0.996620
C	-1.889812	3.127432	-0.996640
H	-5.523214	-1.017426	-0.361077
H	-4.077868	-0.269072	-1.270563
C	-1.653743	3.920081	0.033696
H	-1.469167	4.979483	-0.088578
H	-1.649205	3.540916	1.047454
H	-1.905838	3.519524	-2.006024
H	-2.076886	2.067155	-0.876036

LacTS

Li	2.160008	0.099896	-0.193877
N	4.216178	-0.185532	0.087069
N	1.642900	2.094824	-0.386219
N	1.387418	-0.733830	-1.927929
N	1.139746	-0.737107	1.374998
H	4.746586	0.285158	-0.634745
C	4.582349	-1.603316	0.148544
H	4.448567	0.276166	0.957409
H	0.760318	1.861388	-0.859394
H	2.191246	2.634585	-1.043880
C	1.345760	2.909571	0.795036
H	0.241173	-0.300370	1.115205
C	1.467689	-0.426088	2.765857
H	1.000293	-1.735129	1.278701
H	0.553029	-0.131974	-1.895496
C	0.974794	-2.137546	-1.962378
H	1.871260	-0.502025	-2.786284
H	1.845125	-2.793183	-1.931621
H	0.384420	-2.397693	-2.844213
H	0.365320	-2.352410	-1.086749
H	1.595331	0.649219	2.876373
H	2.407665	-0.900610	3.050866
H	0.701463	-0.742690	3.477658
H	4.328095	-2.079626	-0.795873
H	3.998760	-2.088560	0.927876
H	5.641307	-1.778812	0.349797
H	2.246368	3.065286	1.389757
H	0.615816	2.383210	1.405492
H	0.927385	3.889260	0.551525
C	-1.601866	0.879536	-0.596662
O	-0.803778	1.082866	-1.552265
O	-1.282932	0.494082	0.547536
C	-3.075430	1.162325	-0.895739
C	-4.043133	0.798539	0.172273
H	-3.316833	0.678110	-1.844490
H	-3.132312	2.235726	-1.118142
C	-4.039233	-1.461336	0.219985
H	-5.094747	0.951308	-0.028977
H	-3.731473	0.944951	1.195246
C	-4.964589	-1.950032	1.073912
H	-5.973786	-2.168714	0.752869
H	-4.750111	-2.073277	2.126556
H	-4.232533	-1.461709	-0.844156
H	-3.005811	-1.361263	0.517758

LacP

Li	2.172539	0.088515	-0.210328
N	4.242306	-0.080989	0.068761
N	1.588578	2.014452	-0.693125
N	1.406958	-1.022789	-1.784236
N	1.203031	-0.540475	1.482216
H	4.742843	0.289576	-0.728732
C	4.662373	-1.458057	0.342027
H	4.470076	0.518934	0.851588
H	0.711600	1.682768	-1.116286
H	2.113534	2.467899	-1.430248
C	1.269458	2.986509	0.355867
H	0.286071	-0.184728	1.166186
C	1.520952	-0.007460	2.806239
H	1.104690	-1.546267	1.540738
H	0.556199	-0.444091	-1.830658
C	1.032232	-2.424452	-1.594595

Li	1.835341	0.176631	0.024894
N	3.872941	0.547272	0.319095
N	1.565108	-1.544944	-1.080363
N	0.826585	-0.089042	1.800241
N	0.854951	1.725194	-0.916574
H	3.987823	1.352356	0.921228
C	4.620824	0.725561	-0.927684
H	4.229356	-0.247464	0.834685
H	0.583123	-1.604199	-0.759997
C	2.263104	-2.793926	-0.783286
H	1.528502	-1.405677	-2.082032
H	-0.102664	1.396513	-0.741164
H	0.961778	1.734978	-1.923125
C	1.010772	3.082164	-0.393855
H	0.051907	-0.541409	1.281998
H	0.445702	0.768097	2.180461

Li	-1.938175	-0.080326	-0.307255
N	-1.359109	-0.029849	1.671258
N	-1.672222	1.838935	-1.043732
N	-0.660494	-1.304419	-1.379495
N	-3.910081	-0.786304	-0.493465
H	-0.520590	0.479650	1.335091
C	-0.942887	-1.240209	2.378394
H	-1.848649	0.587017	2.306410
H	-1.668305	1.956608	-2.048547
H	-0.687695	1.769720	-0.744091
C	-2.296567	3.001447	-0.414233
H	-4.221124	-0.647671	-1.446310
C	-4.828995	-0.135626	0.444362
H	-3.897400	-1.786271	-0.338186
H	-0.577906	-0.969469	-2.331418
C	-0.798781	-2.760165	-1.384322

H	1.872939	-0.914498	-2.676275	C	1.276690	-0.953169	2.888953	H	0.217767	-1.040864	-0.924218
H	1.920036	-3.045902	-1.475848	C	-1.823084	-0.620134	-0.544003	H	-0.875612	-3.119906	-0.359475
H	0.439007	-2.833010	-2.416325	O	-1.807874	0.695594	-0.388092	H	0.038366	-3.280093	-1.857099
H	0.438491	-2.515225	-0.687028	O	-0.985107	-1.377938	0.068000	H	-1.711242	-3.050962	-1.905416
H	1.603807	1.076417	2.750181	C	-3.151978	-1.189676	-0.997995	H	-4.823239	0.937287	0.264284
H	2.480621	-0.393717	3.152564	C	-4.276502	-0.185399	-0.758383	H	-4.474336	-0.299120	1.459342
H	0.770012	-0.242330	3.564568	H	-3.118835	-1.499140	-2.046386	H	-5.859145	-0.492126	0.374389
H	4.411396	-2.084520	-0.511232	H	-3.333609	-2.097662	-0.416292	H	-0.280031	-1.814130	1.733824
H	4.109599	-1.835580	1.199538	H	-5.244594	-0.674380	-0.874186	H	-1.804690	-1.864290	2.620449
H	5.730226	-1.563384	0.545510	H	-4.230650	0.614881	-1.498731	H	-0.399175	-1.039262	3.304976
H	2.167266	3.261044	0.910592	C	-2.957792	1.310324	0.777343	H	-2.250714	2.889910	0.667652
H	0.562524	2.532640	1.046394	C	-4.166989	0.421766	0.645292	H	-3.347292	3.071606	-0.697571
H	0.814695	3.903490	-0.027007	H	-2.444008	1.279801	1.730695	H	-1.813619	3.948901	-0.666496
C	-1.608650	0.684144	-0.675310	H	-3.083788	2.319039	0.403077	C	4.343694	-0.603669	-0.328642
O	-0.828624	0.766710	-1.664618	H	-4.116267	-0.391311	1.372829	C	3.135905	-1.302346	0.269845
O	-1.259802	0.461431	0.504125	H	-5.072415	0.988329	0.876715	C	4.379790	0.851934	0.117865
C	-3.089322	0.921511	-0.966620	H	3.308326	-2.732126	-1.089737	H	4.276737	-0.655839	-1.418142
C	-4.052914	0.456660	0.112238	H	1.821594	-3.669579	-1.265823	H	5.252962	-1.130940	-0.031938
H	-3.316441	0.459791	-1.928466	H	2.244639	-2.970515	0.291042	C	3.040363	1.523017	-0.169319
H	-3.193851	1.997490	-1.125294	H	2.017429	3.451624	-0.590982	H	5.192793	1.385762	-0.377137
C	-4.137051	-1.062467	0.230084	H	0.871205	3.071369	0.686182	H	4.576809	0.891858	1.191774
H	-5.049572	0.852176	-0.096144	H	0.299857	3.798913	-0.812377	H	2.918328	1.643967	-1.259994
H	-3.736122	0.867021	1.071287	H	4.473673	-0.147853	-1.559340	H	2.998294	2.520875	0.264186
H	-4.443668	-1.492570	-0.728813	H	5.693658	0.872318	-0.784528	C	1.870972	0.733419	0.356114
C	-5.043276	-1.529807	1.304597	H	4.225486	1.586873	-1.462318	O	1.930130	-0.645541	-0.067481
H	-3.121820	-1.440900	0.410553	H	1.629052	-1.898158	2.478129	O	0.683774	1.217784	0.272621
H	-5.202921	-0.927860	2.188169	H	0.494879	-1.186120	3.616570	H	3.234409	-1.339517	1.361566
H	-5.460366	-2.526220	1.292954	H	2.109294	-0.495070	3.424365	H	3.049973	-2.325017	-0.099602
		OHTS				OHEtp					
Li	1.449774	0.006354	-0.385231	Li	0.798381	-0.828744	-0.463972				
N	3.518933	-0.036876	-0.731080	N	2.666731	0.002758	-0.153241				
N	0.520310	1.449638	-1.556132	N	0.145437	-0.857836	-2.462426				
N	0.507147	-1.773533	-0.900733	N	0.316013	-2.690276	0.374418				
N	1.107234	0.293611	1.623843	N	1.276145	2.418924	1.107220				
H	3.719047	-0.151955	-1.716450	H	3.134864	0.209189	-1.026400				
C	4.192749	-1.078995	0.049677	C	3.593205	-0.668321	0.759143				
H	3.873301	0.876319	-0.475481	H	2.375376	0.900384	0.247994				
H	-0.369468	0.952292	-1.650224	H	-0.805647	-1.055116	-2.166352				
H	0.887662	1.559916	-2.493079	H	0.407770	-1.562982	-3.137790				
C	0.260136	2.769585	-0.970838	C	0.211215	0.478461	-3.058746				
H	0.097219	0.374315	1.466273	H	0.491411	1.781442	0.967944				
C	1.603438	1.441665	2.382887	C	1.071193	3.662890	0.374717				
H	1.235283	-0.551275	2.166326	H	1.355245	2.599133	2.098569				
H	-0.379071	-1.344871	-1.178619	H	-0.657202	-2.544875	0.122867				
C	0.245040	-2.746207	0.165448	C	0.449497	-2.703683	1.833523				
H	0.864940	-2.251925	-1.717884	H	0.603096	-3.577096	-0.017231				
H	1.182532	-3.142189	0.555875	H	1.494461	-2.844589	2.104519				
H	-0.372705	-3.587158	-0.156249	H	-0.138130	-3.484734	2.321963				
H	-0.278617	-2.245267	0.976505	H	0.126826	-1.739474	2.220287				
H	1.439246	2.352718	1.811093	H	0.981675	3.443685	-0.688710				
H	2.676423	1.346957	2.551816	H	1.932780	4.318271	0.500358				
H	1.118212	1.566504	3.353528	H	0.176471	4.218772	0.672193				
H	3.800313	-2.052116	-0.237761	H	3.872567	-1.643124	0.361261				
H	3.970277	-0.933783	1.104471	H	3.097310	-0.832785	1.713775				
H	5.277319	-1.093694	-0.075832	H	4.508732	-0.102707	0.950895				
H	1.198380	3.286450	-0.769835	H	1.237880	0.702895	-3.345051				
H	-0.267310	2.634924	-0.029582	H	-0.097683	1.206830	-2.312189				
H	-0.352384	3.411775	-1.607481	H	-0.422235	0.600173	-3.940693				
C	-2.390445	0.118179	-0.097485	C	-1.786963	0.078681	0.262476				
O	-1.941878	-0.181981	-1.330503	O	-2.181955	-1.063720	-0.451918				
O	-1.644809	0.386278	0.836347	O	-0.526085	0.241908	0.302647				
C	-3.847765	-0.069726	-0.164988	C	-2.771318	0.873895	0.824913				
C	-4.610905	-0.549712	0.922413	C	-4.145204	0.694689	0.746993				
H	-3.122878	-0.607462	-1.390774	H	-3.139800	-1.138746	-0.393102				
H	-4.311055	0.677158	-0.806178	H	-2.391948	1.718282	1.384831				
H	-4.143699	-1.091697	1.731667	H	-4.615953	-0.099845	0.180831				
H	-5.687638	-0.477992	0.922841	H	-4.818723	1.373083	1.245397				

Table S8. Harmonic vibrational frequencies (cm^{-1}) for the reactants, products, and intermediates of the $Li(NH_3)_4 + CO_2 + 2\ H_2 \rightarrow Li(NH_3)_4 + CH_2(OH)_2$ reaction pathway.

$Li(NH_3)_4$			CO_2			H_2			Formic Acid		
58.2	324.3	1646.1	686.2			4406.9			527.6		
64.5	407.3	1646.1	686.2						670.6		
64.8	407.4	1646.1	1399.5						1048.8		
65.0	503.6	3407.9	2450.6						1128.8		
74.4	503.8	3408.0							1282.7		
74.5	504.2	3408.0							1424.6		
76.2	1147.8	3425.9							1903.1		
76.4	1147.8	3527.4							2995.4		
76.5	1147.8	3527.4							3843.7		
239.0	1159.1	3527.4									
315.2	1638.5	3530.4									
315.3	1638.5	3530.4									
315.6	1644.3	3534.8									
324.1	1644.3	3534.8									
324.2	1644.3	3534.9									
Methyldiol			CO_2r			eTS1			CO_2p		
357.4			15.4	329.1	1643.2	-796.2	323.4	1651.3	11.7	350.3	1665.6
373.6			22.2	342.9	1647.2	19.7	329.6	1653.0	30.4	377.0	1666.0
564.8			38.4	346.6	1647.6	39.7	345.8	1657.2	41.9	397.0	1691.7
1014.9			51.5	413.6	1653.5	51.3	351.8	1658.7	63.4	423.5	1701.7
1062.9			53.5	423.3	1655.0	58.8	383.7	1658.7	69.2	500.1	1705.1
1093.0			64.5	499.6	2428.3	69.0	418.5	2270.2	107.1	556.7	1723.5
1210.9			75.4	502.0	3390.9	82.6	450.5	3407.5	113.8	564.1	3212.3
1375.7			79.7	513.1	3404.3	84.7	513.0	3413.3	122.9	575.8	3270.2
1393.6			85.9	638.3	3421.4	88.8	526.5	3421.9	141.3	645.4	3307.1
1452.5			86.0	641.9	3430.1	92.3	565.1	3448.1	184.8	747.5	3501.7
1536.4			88.6	1153.1	3505.1	116.4	1142.9	3507.2	225.0	1130.0	3539.1
3057.5			95.1	1156.2	3513.5	117.7	1159.3	3519.8	228.8	1213.2	3543.1
3103.2			105.9	1161.1	3514.8	127.4	1168.0	3522.7	237.0	1233.5	3544.5
3846.3			127.1	1168.5	3529.1	136.6	1184.0	3544.0	249.8	1250.9	3601.1
3847.2			237.6	1389.8	3530.7	157.0	1217.4	3546.4	255.8	1346.3	3605.2
			317.2	1636.4	3532.3	209.2	1643.3	3549.7	265.7	1649.3	3605.8
			320.8	1636.6	3553.3	238.7	1645.1	3564.7	316.8	1653.8	3612.9
			326.1	1643.1	3554.2	315.9	1649.4	3565.6	321.7	1665.4	3613.3
H_2r1			CHTS1			CHp1			OHTS1		
14.8	323.0	1665.6	-485.1	352.9	1654.9	5.2	323.2	1660.9	-1431.1	346.3	1666.3
28.8	348.8	1665.9	13.5	375.0	1665.7	22.9	354.6	1665.3	24.8	374.4	1666.5
30.7	376.6	1666.2	26.8	378.8	1666.0	44.5	381.1	1665.9	29.9	382.7	1669.7
32.7	394.0	1690.9	44.0	395.9	1668.5	57.7	396.8	1672.0	48.5	406.6	1685.6
42.5	398.6	1701.2	55.9	427.5	1695.4	63.3	430.9	1697.2	57.6	476.9	1694.8
64.9	423.2	1704.7	67.9	507.4	1703.0	66.5	513.1	1711.9	69.5	533.4	1711.2
70.9	423.6	1724.2	75.2	564.4	1709.5	108.3	564.8	1719.9	83.5	560.2	1739.0
108.5	496.4	3228.0	109.0	571.4	1725.3	113.2	576.4	2922.6	106.3	565.2	3023.9
114.9	553.2	3285.2	113.8	574.1	3192.0	127.6	579.5	3172.4	111.0	625.9	3258.5
122.9	565.1	3322.4	125.7	655.9	3260.1	140.0	659.6	3225.2	117.9	669.7	3390.3
145.4	575.8	3501.5	187.3	783.8	3296.6	155.5	773.3	3269.0	156.5	802.5	3404.7
178.6	643.3	3540.0	204.8	1103.7	3501.8	195.6	1090.2	3502.2	181.6	1090.3	3500.3
185.0	748.2	3543.5	235.3	1131.3	3539.0	233.3	1127.3	3539.2	193.7	1138.3	3535.5
221.7	1132.0	3544.8	238.4	1210.7	3545.7	240.3	1213.4	3545.1	214.1	1198.2	3545.6
224.7	1213.0	3601.6	250.2	1233.6	3546.8	247.5	1239.4	3546.1	227.2	1217.7	3546.1
235.3	1232.0	3604.8	266.1	1258.0	3600.7	252.6	1262.2	3601.1	240.1	1258.8	3595.4
246.9	1247.3	3605.7	267.9	1331.5	3607.0	274.3	1394.7	3607.8	253.6	1321.8	3599.3
250.9	1345.6	3612.4	297.6	1385.3	3607.3	279.4	1408.9	3607.9	315.9	1411.3	3599.4
263.3	1649.5	3612.8	318.0	1479.5	3612.9	296.2	1638.9	3613.9	321.0	1653.5	3609.9
317.7	1654.2	4340.8	324.2	1651.6	3613.0	317.7	1650.2	3614.0	325.5	1658.0	3611.3
OHp1			eTS2			rFA			H_2r2		
22.7	428.0	1688.9	-784.8	405.7	1687.0	19.2	410.9	1706.5	19.9	362.0	1647.7

36.1	456.9	1825.7	30.7	454.3	1699.6	42.8	529.1	1722.7	27.9	384.6	1662.4
37.0	515.7	3058.3	36.1	475.5	3112.3	57.5	541.2	2908.7	40.2	392.6	1665.0
50.4	540.4	3330.7	38.2	482.0	3260.6	62.3	557.3	3113.1	47.0	412.6	1666.9
64.9	546.7	3338.7	48.9	540.6	3379.4	70.2	570.7	3154.3	59.0	437.0	1674.4
73.5	567.1	3437.7	66.4	551.6	3399.0	92.8	583.6	3263.3	63.8	461.3	1705.6
78.9	691.4	3440.9	92.3	624.7	3442.7	104.3	654.8	3504.3	72.5	528.7	1721.5
87.3	1047.7	3457.2	105.3	647.3	3476.3	109.3	897.1	3541.3	95.3	539.5	2913.7
97.3	1143.5	3461.9	108.0	1003.3	3507.1	122.6	979.8	3541.9	105.2	558.1	3132.3
105.8	1153.4	3510.2	116.9	1135.9	3547.7	182.8	1106.7	3546.6	110.8	569.7	3173.1
116.2	1161.3	3538.8	150.4	1178.9	3551.1	214.2	1165.9	3607.2	123.5	583.3	3269.8
127.9	1192.7	3547.9	161.1	1191.9	3589.0	224.4	1211.1	3607.9	181.1	654.6	3504.0
144.7	1204.5	3570.6	181.1	1197.6	3595.3	229.4	1221.2	3610.8	208.0	901.5	3541.6
159.7	1261.0	3572.8	196.5	1238.3	3603.1	268.9	1254.8	3618.0	209.5	980.6	3542.1
190.9	1419.7	3583.0	220.3	1365.6	3606.6	286.3	1315.8	3619.5	223.2	1109.5	3546.3
235.1	1630.1	3592.5	231.6	1577.2	3719.3	296.5	1464.3	3860.1	230.4	1167.7	3607.3
318.1	1639.3		255.3	1628.5		299.6	1642.9		265.9	1211.1	3607.6
325.9	1645.7		320.3	1637.1		302.8	1647.0		282.9	1222.1	3610.0
337.4	1654.4		328.5	1652.1		307.8	1661.7		295.4	1254.3	3617.4
347.2	1658.1		337.6	1658.2		363.4	1664.8		301.0	1318.0	3618.8
361.5	1661.8		367.9	1660.6		385.0	1666.7		303.7	1462.5	3859.8
373.0	1663.9		377.6	1671.2		392.5	1674.7		308.2	1643.7	4300.3
CHTS2			CHp2			OHTS2			OHp2		
-432.5	473.9	1671.5	15.6	389.4	1654.6	-517.4	377.4	1654.3	21.5	373.5	1646.1
81.1	478.7	1678.2	29.1	407.4	1663.8	19.2	388.1	1663.1	42.2	404.8	1647.8
91.8	490.0	1683.5	50.6	413.3	1665.5	31.1	412.2	1664.0	42.8	441.7	1650.9
103.5	508.0	1685.3	61.2	463.2	1667.4	52.6	495.6	1666.3	61.7	444.7	1653.6
115.0	546.7	1716.9	62.0	510.3	1695.8	60.6	522.7	1685.4	67.3	507.8	1675.2
121.1	584.8	1721.9	90.1	540.5	1705.4	69.6	548.4	1699.0	69.7	518.4	1679.2
148.1	605.0	1741.1	98.9	561.2	1717.5	91.7	560.7	1708.7	73.3	532.7	3077.1
150.3	642.9	1848.5	106.9	566.4	2892.9	99.7	571.5	2921.2	76.0	566.8	3129.5
161.4	658.3	2759.1	113.1	580.5	2917.2	105.8	578.8	2937.6	93.1	1007.9	3361.1
214.2	724.6	2857.0	183.8	656.9	3117.3	116.2	640.2	3220.1	99.6	1056.0	3420.7
217.0	809.7	3009.6	188.6	862.5	3178.5	153.9	888.7	3294.6	105.7	1074.0	3431.3
242.9	1122.3	3235.4	206.5	1108.3	3349.5	180.7	1106.5	3370.0	121.2	1148.3	3436.9
293.8	1160.7	3394.9	214.1	1110.1	3503.8	191.3	1118.5	3502.8	138.5	1161.4	3467.2
307.4	1225.1	3422.6	232.6	1152.4	3541.4	210.2	1151.1	3540.6	186.2	1166.3	3483.2
334.5	1243.4	3423.0	240.5	1213.9	3542.2	218.6	1208.7	3543.4	198.8	1176.9	3532.2
363.9	1304.1	3428.1	260.4	1230.0	3547.4	231.4	1221.0	3549.0	237.7	1198.8	3534.0
365.6	1314.9	3478.3	269.4	1259.7	3605.3	241.0	1246.4	3604.8	295.0	1393.1	3539.3
375.9	1318.1	3480.0	297.3	1266.8	3606.2	289.4	1271.3	3605.7	322.0	1397.8	3547.4
401.3	1344.0	3481.5	304.5	1296.8	3606.6	308.8	1288.1	3606.0	325.3	1443.4	3555.0
408.3	1405.6	3488.6	308.7	1438.3	3616.5	318.3	1443.0	3614.3	326.5	1526.4	3559.6
411.0	1463.2	3490.6	352.5	1539.7	3619.3	348.7	1532.9	3617.6	336.2	1628.4	3706.0
437.9	1659.7	3716.8	379.8	1646.4	3842.8	351.2	1646.1	3842.4	357.3	1631.4	3829.8

Table S9. Harmonic vibrational frequencies (cm^{-1}) for the reactants, products, and intermediates of the $Li(NH_2CH_3)_4 + CO_2 + 2\ H_2 \rightarrow Li(NH_2CH_3)_4 + CH_2(OH)_2$ reaction pathway.

$Li(NH_2CH_3)_4$			CO_2r			eTS1			CO_2p		
31.6	993.0	1651.7	14.6	554.9	1511.7	-382.4	507.8	1511.2	18.5	603.8	1513.1
32.0	997.9	3038.8	23.8	581.9	1522.2	19.8	536.7	1522.5	23.5	745.3	1523.6
33.4	1001.9	3039.1	25.6	958.1	1523.8	26.3	948.6	1524.9	41.1	934.7	1528.4
34.3	1058.2	3041.3	31.9	964.4	1526.6	31.6	971.4	1526.4	49.9	984.7	1529.5
45.3	1060.4	3041.9	33.8	969.3	1527.8	33.3	975.3	1528.5	51.8	987.2	1531.2
56.9	1062.5	3099.9	37.4	989.8	1617.5	39.0	989.2	1621.3	69.3	996.7	1663.5
65.3	1063.5	3100.1	40.4	993.5	1640.4	51.9	996.4	1641.2	77.3	999.1	1680.1
75.5	1207.5	3105.7	48.4	998.2	1650.3	54.0	997.9	1656.4	79.7	1045.3	1695.7
75.7	1207.7	3106.5	53.9	998.7	1662.7	55.6	1005.2	1667.7	86.7	1058.0	1697.5
97.1	1215.4	3123.7	65.1	1004.9	2423.6	59.8	1013.2	2353.3	101.8	1065.8	1711.6
129.2	1218.4	3124.1	68.8	1057.6	3038.1	65.4	1058.5	3040.4	103.5	1067.8	3032.8
135.0	1351.5	3132.5	73.4	1060.0	3040.5	70.9	1060.8	3040.8	110.6	1072.8	3034.6
135.1	1352.7	3133.0	82.9	1063.3	3041.2	81.4	1064.6	3041.2	133.3	1081.4	3035.9
166.0	1353.9	3381.4	97.2	1066.5	3042.5	95.8	1068.2	3042.5	138.2	1089.0	3040.1
168.7	1355.4	3389.4	111.0	1207.4	3099.1	98.5	1203.9	3099.8	140.5	1199.8	3083.7
181.6	1457.8	3430.2	114.6	1210.3	3102.5	125.4	1212.9	3100.3	155.2	1228.6	3086.5
208.4	1458.2	3448.2	133.2	1216.1	3103.4	130.5	1218.9	3102.0	164.9	1235.6	3087.7
233.6	1465.2	3450.8	147.8	1220.0	3107.0	137.5	1223.0	3108.1	170.5	1241.0	3108.5
355.5	1467.9	3456.6	160.9	1352.4	3121.8	146.2	1297.5	3123.1	177.4	1349.0	3122.3
374.7	1504.4	3536.2	179.4	1353.0	3129.9	166.8	1352.6	3130.1	197.7	1353.0	3128.0
402.5	1504.5	3536.4	187.5	1354.0	3130.9	173.7	1354.3	3132.9	215.3	1376.7	3135.7
437.4	1507.6		199.6	1358.7	3133.8	186.7	1356.4	3135.5	229.7	1380.9	3136.9
475.6	1509.4		239.9	1379.8	3375.5	210.5	1362.4	3337.8	238.0	1397.0	3284.9
491.3	1521.9		372.4	1457.7	3394.1	236.0	1458.1	3377.6	248.4	1467.2	3311.5
496.2	1522.1		392.6	1460.9	3430.2	366.6	1461.8	3449.6	374.0	1468.3	3343.4
956.9	1524.2		399.3	1466.0	3452.6	373.2	1467.4	3483.0	405.7	1469.0	3523.9
959.9	1526.5		441.0	1468.9	3460.6	394.7	1470.7	3488.4	456.8	1471.7	3551.4
964.3	1618.2		463.9	1504.1	3495.9	420.3	1504.0	3493.9	507.8	1508.6	3553.7
990.9	1638.3		497.4	1504.5	3540.4	442.4	1507.2	3561.1	521.0	1509.6	3554.7
991.2	1645.6		514.5	1507.8	3559.6	491.1	1508.5	3561.7	543.4	1512.0	3592.0
H_2r1			CHTS1			CHp1			OHTS1		
14.3	507.0	1512.0	-505.6	561.0	3087.7	19.1	556.3	1512.4	-1398.0	585.1	1511.3
23.2	519.9	1513.1	20.1	607.5	3111.1	22.0	611.7	1513.5	28.2	668.9	1513.7
24.9	543.3	1523.7	33.1	780.3	3122.0	37.3	770.3	1523.2	28.7	810.1	1523.8
28.4	602.8	1528.3	43.4	936.4	3127.7	42.3	932.5	1528.3	37.7	942.4	1528.0
42.2	746.3	1529.6	46.5	984.9	3135.8	46.2	986.0	1529.8	41.7	982.0	1530.0
49.0	936.2	1531.1	56.0	987.9	3139.9	49.7	987.4	1531.7	51.0	988.8	1531.5
53.2	984.5	1663.7	62.4	998.7	3271.9	53.9	999.1	1659.5	56.0	998.5	1663.3
69.1	987.2	1680.0	74.5	1001.6	3306.1	71.2	1000.8	1663.8	64.8	1002.8	1673.9
77.5	996.8	1695.7	81.7	1047.7	3340.2	83.2	1053.8	1685.4	70.7	1023.7	1687.3
79.7	999.1	1697.1	89.3	1060.6	3524.0	86.6	1064.6	1705.7	79.8	1048.2	1702.7
86.3	1044.5	1711.3	96.5	1064.2	3551.5	92.5	1067.0	1706.5	89.0	1060.8	1731.2
100.7	1057.4	3034.1	103.8	1068.9	3552.3	103.9	1072.3	2803.6	93.2	1065.4	3025.2
102.3	1065.4	3035.4	105.3	1074.0	3554.8	106.8	1076.9	3029.7	99.2	1070.4	3036.0
110.3	1067.4	3036.6	117.3	1084.0	3591.9	115.5	1085.3	3030.9	105.9	1075.9	3039.3
132.7	1072.5	3040.6	126.1	1092.9	1511.2	122.8	1087.1	3032.0	122.5	1081.7	3041.4
137.7	1081.1	3084.8	141.1	1110.1	1511.4	134.5	1099.8	3038.9	130.1	1091.3	3042.8
140.3	1087.9	3087.5	154.6	1201.3	1513.5	140.7	1199.2	3079.9	137.4	1202.6	3087.7
156.4	1200.3	3088.8	164.4	1229.6	1525.2	142.3	1231.6	3082.4	144.1	1223.8	3092.7
164.2	1228.4	3108.8	169.9	1241.7	1529.1	157.8	1243.0	3083.1	163.9	1232.7	3097.8
169.8	1236.6	3122.2	180.7	1243.2	1529.8	171.3	1246.9	3108.3	167.1	1245.7	3110.6
175.9	1240.4	3127.9	198.6	1333.2	1531.9	173.6	1352.7	3120.2	183.8	1323.8	3118.1
186.2	1350.4	3136.1	211.1	1353.2	1663.7	181.4	1381.0	3126.2	208.0	1353.5	3120.1
197.1	1353.0	3137.1	218.5	1378.5	1682.5	202.1	1384.5	3134.8	211.3	1368.5	3135.1
214.7	1376.3	3290.5	237.6	1383.2	1701.3	219.6	1388.3	3137.1	220.1	1382.2	3139.0
228.1	1381.3	3318.0	252.4	1386.4	1702.2	234.5	1399.4	3230.1	245.0	1391.7	3306.7
237.1	1396.5	3348.8	298.3	1399.8	1705.8	246.1	1408.8	3261.8	318.1	1411.7	3424.4
247.1	1467.7	3523.7	378.2	1467.3	3033.7	259.5	1466.6	3305.7	376.0	1467.1	3438.1
374.6	1468.3	3551.4	381.1	1468.5	3034.6	373.6	1467.4	3524.9	405.6	1469.7	3521.8
393.6	1469.2	3552.7	412.1	1468.6	3035.6	412.2	1468.6	3552.4	442.8	1470.1	3546.2
405.9	1471.9	3554.4	441.6	1470.1	3040.9	460.6	1471.4	3553.1	471.6	1473.4	3547.8
409.6	1508.3	3591.5	504.8	1472.8	3086.1	510.8	1508.3	3554.2	510.9	1504.2	3555.9
456.0	1509.4	4341.0	517.4	1508.5	3087.0	528.0	1509.5	3593.3	550.7	1508.7	3589.0
OHp1			eTS2			rFA			H_2r2		
26.1	699.8	1511.8	-793.6	581.6	1511.6	27.6	605.7	1508.9	24.6	509.6	1507.0
31.3	942.8	1524.2	27.6	649.8	1525.7	30.9	891.4	1511.9	28.3	563.8	1509.0
43.5	980.1	1526.1	33.8	942.9	1526.6	37.0	927.3	1522.7	30.8	577.3	1512.0
47.3	987.2	1527.1	38.9	977.8	1528.9	41.0	977.0	1525.1	37.1	605.5	1522.7
49.3	990.4	1529.2	50.8	988.5	1530.5	47.4	986.0	1527.2	40.8	895.6	1525.2
56.7	996.0	1636.9	57.7	989.1	1595.4	56.5	993.2	1528.9	42.8	928.8	1527.3
71.0	999.5	1651.7	62.9	992.5	1659.8	66.4	996.2	1663.4	48.3	977.6	1529.1
72.8	1018.1	1662.3	69.2	1001.2	1667.4	70.5	1007.9	1669.6	58.4	985.8	1663.4
73.6	1033.1	1687.7	76.7	1017.6	1670.4	78.8	1036.2	1701.6	68.7	992.9	1669.4
81.1	1058.1	1805.6	83.2	1027.6	1694.0	98.6	1065.2	1715.8	73.5	996.7	1700.7

89.1	1058.5	3015.3	91.9	1051.4	3035.5	102.0	1068.4	2909.3	79.4	1007.8	1715.1
96.5	1066.2	3038.1	96.0	1059.1	3036.0	104.7	1076.9	3023.9	99.5	1036.4	2913.7
102.4	1071.1	3040.1	104.8	1065.6	3039.6	115.7	1082.6	3025.7	102.5	1063.7	3025.3
115.1	1073.1	3041.6	113.5	1073.1	3040.9	135.3	1085.5	3027.0	104.7	1067.9	3027.0
123.1	1163.1	3042.1	126.5	1077.0	3091.6	139.2	1095.3	3036.6	115.1	1076.3	3028.0
134.6	1202.4	3063.1	129.2	1202.7	3092.4	141.9	1167.5	3073.9	135.6	1082.3	3037.3
136.4	1221.2	3095.4	140.3	1223.6	3093.9	150.4	1197.5	3077.9	139.1	1084.8	3075.3
144.4	1227.7	3096.8	151.5	1227.8	3108.3	156.2	1231.8	3082.8	141.6	1094.4	3079.4
148.5	1230.5	3101.0	168.8	1228.7	3116.1	173.2	1235.0	3104.8	150.6	1168.8	3083.7
170.7	1265.5	3108.4	173.2	1238.7	3118.0	195.4	1248.7	3106.6	155.7	1197.9	3105.4
177.6	1353.3	3118.5	185.3	1352.4	3124.3	210.0	1315.2	3111.6	172.8	1232.1	3107.0
191.6	1356.7	3128.0	189.5	1357.2	3136.8	218.9	1351.6	3117.0	195.6	1235.0	3112.5
218.2	1360.6	3128.5	205.4	1358.3	3141.3	239.9	1359.5	3136.4	208.2	1248.8	3117.6
236.6	1376.7	3138.4	230.5	1371.9	3327.8	268.6	1377.3	3169.3	210.9	1317.6	3136.5
367.5	1415.3	3347.5	246.0	1383.0	3365.4	306.2	1388.5	3205.3	217.7	1351.6	3184.5
396.5	1463.9	3379.5	381.9	1462.5	3448.8	370.8	1463.9	3330.8	240.0	1359.5	3219.3
413.8	1465.0	3437.0	405.6	1467.0	3506.1	409.5	1467.9	3526.5	266.9	1377.0	3333.0
455.2	1467.3	3503.2	438.8	1469.8	3509.0	457.1	1468.8	3554.5	306.2	1388.2	3526.2
498.8	1472.4	3508.4	477.1	1471.1	3513.8	487.3	1471.5	3556.2	371.9	1463.0	3555.0
518.8	1506.6	3524.7	491.6	1506.4	3545.6	509.2	1472.7	3557.0	411.4	1468.0	3555.5
542.4	1508.6	3550.3	502.6	1508.0	3558.9	564.6	1506.7	3595.3	438.0	1468.7	3556.9
580.3	1509.1	3576.6	537.6	1509.6	3577.3	576.9	1507.0	3857.8	458.4	1471.0	3594.7
									462.9	1472.3	3857.3
									487.8	1506.8	4300.1
CHTS2			CHp2			OHTS2			OHp2		
-426.6	656.1	1518.8	19.6	590.6	1510.7	-468.5	607.2	1510.7	15.6	940.5	1511.7
61.9	709.0	1520.1	25.9	614.2	1512.3	15.7	632.2	1512.3	26.6	985.6	1520.0
68.7	805.8	1523.2	35.7	905.8	1523.6	27.6	922.4	1521.7	32.2	987.1	1523.1
87.2	1000.0	1529.9	45.1	932.6	1524.5	33.5	934.0	1523.9	42.7	989.8	1524.4
93.6	1026.8	1531.8	51.2	987.6	1526.9	44.0	987.2	1524.6	44.3	999.7	1526.6
95.9	1028.3	1534.8	67.9	990.3	1527.3	50.3	989.8	1526.8	48.7	1005.8	1530.1
103.0	1035.7	1537.8	69.8	999.3	1530.8	65.7	997.9	1530.6	60.0	1012.8	1621.0
112.5	1039.3	1678.9	75.8	1005.6	1663.0	69.7	1005.2	1663.2	63.1	1026.2	1662.2
132.0	1041.6	1693.0	78.7	1040.0	1696.5	75.8	1034.3	1692.9	70.4	1040.0	1685.2
140.1	1043.6	1711.8	88.0	1043.5	1711.7	79.2	1042.1	1710.0	71.4	1041.6	1694.3
149.1	1049.6	1733.1	99.5	1057.5	1722.7	88.3	1051.1	1717.6	91.1	1058.0	3036.7
160.6	1052.9	1861.4	114.1	1065.7	2945.3	98.9	1065.4	2963.8	102.1	1065.8	3037.4
165.9	1095.2	2763.5	123.2	1074.7	2966.1	112.1	1073.5	2991.6	107.4	1072.6	3039.4
175.7	1115.1	2852.1	130.5	1076.1	3025.9	127.4	1074.5	3027.7	118.4	1074.0	3041.4
177.6	1117.1	2923.4	133.8	1079.8	3035.3	131.7	1077.5	3036.0	131.9	1083.4	3054.9
209.1	1132.8	2923.8	137.5	1098.1	3036.0	137.2	1093.8	3038.3	136.1	1202.0	3091.8
230.8	1168.4	2926.0	143.6	1195.9	3039.1	137.8	1183.7	3039.6	139.9	1205.2	3093.9
244.2	1235.0	2937.1	152.4	1200.0	3075.7	140.1	1200.3	3079.5	146.9	1226.3	3097.4
257.6	1247.9	2960.3	163.6	1233.8	3087.6	151.8	1230.4	3090.2	159.3	1228.4	3108.8
265.1	1273.7	2970.8	178.2	1239.1	3089.6	170.0	1237.7	3091.3	168.0	1233.2	3116.5
322.1	1289.8	2978.2	205.3	1247.1	3106.9	177.7	1244.9	3110.5	184.0	1353.6	3118.4
339.9	1305.8	2991.3	213.8	1256.1	3110.5	204.8	1256.2	3114.5	196.5	1357.6	3122.8
344.7	1315.9	2998.2	221.7	1354.1	3112.9	215.1	1354.2	3116.4	215.6	1368.9	3137.5
348.2	1374.4	3000.6	232.5	1355.9	3116.2	225.1	1363.0	3126.0	238.5	1377.6	3141.6
349.3	1402.3	3006.5	261.9	1381.9	3126.1	233.6	1378.1	3140.1	373.5	1393.1	3307.1
354.2	1408.1	3027.5	364.2	1388.1	3140.0	296.2	1386.6	3151.5	400.5	1420.5	3413.6
412.1	1409.5	3036.8	391.0	1399.8	3255.7	364.8	1396.2	3311.8	440.2	1437.7	3432.4
428.9	1428.3	3245.6	417.5	1423.2	3337.4	393.8	1426.8	3346.5	450.2	1456.8	3443.3
444.0	1465.3	3399.6	463.8	1465.4	3524.2	415.0	1465.5	3523.8	470.7	1465.6	3508.2
467.5	1477.6	3425.6	466.9	1467.7	3544.1	463.0	1467.8	3544.0	473.4	1468.8	3511.1
475.4	1481.8	3426.2	487.4	1471.2	3546.7	496.1	1471.2	3546.7	490.4	1472.2	3530.3
543.0	1483.9	3436.0	502.2	1472.4	3552.5	515.7	1472.5	3552.1	527.3	1503.6	3545.7
557.9	1485.3	3458.8	525.1	1503.6	3593.1	552.8	1503.1	3592.5	559.2	1506.3	3580.2
635.9	1514.8	3719.5	560.5	1504.0	3828.6	562.0	1504.0	3827.8	577.7	1509.5	3588.3

Table S10. Harmonic vibrational frequencies (cm^{-1}) for the reactants, products, and intermediates of the $Li(NH_2CH_2CH_3)_4 + CO_2 + 2\ H_2 \rightarrow Li(NH_2CH_2CH_3)_4 + CH_2(OH)_2$ reaction pathway.

$Li(NH_2CH_2CH_3)_4$			CO_2r			eTS1			CO_2p		
21.0	988.6	1530.0	13.2	793.3	1497.5	-2.9	904.1	1512.7	13.5	801.4	1500.4
26.6	995.9	1614.2	18.1	814.7	1498.9	10.5	904.8	1513.8	18.3	813.9	1502.7
28.7	1018.8	1635.3	23.3	901.1	1499.2	13.4	969.4	1517.5	27.8	902.4	1502.8
34.1	1023.0	1647.9	25.8	903.3	1501.1	17.9	1002.3	1518.8	31.1	904.6	1504.0
36.4	1026.4	1655.9	31.3	903.9	1501.7	22.9	1004.5	1620.8	33.8	907.2	1505.7
37.6	1030.2	3031.2	35.6	905.1	1509.4	27.5	1019.0	1643.0	44.4	907.9	1517.0
43.3	1033.8	3044.2	36.3	981.1	1513.0	29.1	1023.5	1657.6	49.4	960.4	1517.4
45.9	1084.2	3046.0	38.9	995.1	1516.9	31.2	1032.6	1665.0	53.3	1014.0	1519.1
55.6	1086.8	3046.1	41.7	999.7	1518.4	35.9	1036.4	3044.0	61.7	1018.7	1537.2
72.9	1089.4	3046.5	44.1	1021.6	1531.4	43.2	1040.6	3044.4	62.8	1027.2	1661.7
74.7	1109.9	3056.0	50.3	1025.0	1614.8	56.4	1084.3	3046.3	70.6	1029.3	1674.7
86.6	1169.5	3061.5	51.4	1027.8	1640.1	68.3	1085.9	3046.8	77.3	1055.8	1691.1
94.9	1172.2	3063.6	58.4	1030.0	1654.0	70.9	1087.6	3051.6	89.8	1081.4	1693.7
111.5	1180.7	3082.9	62.1	1035.0	1658.8	73.7	1091.5	3054.7	91.0	1084.1	1712.0
127.5	1188.6	3083.1	73.5	1084.1	2416.7	79.8	1167.3	3056.1	98.3	1088.1	3024.6
141.0	1279.7	3089.5	81.8	1087.3	3029.3	96.2	1179.1	3066.7	111.4	1090.9	3038.6
163.1	1280.1	3090.2	90.2	1090.3	3044.1	104.2	1181.4	3082.8	130.0	1099.0	3042.1
181.6	1283.6	3109.3	100.5	1109.0	3046.2	110.2	1184.6	3085.5	130.9	1119.8	3043.0
255.7	1285.1	3111.5	110.8	1170.0	3047.2	114.0	1279.3	3092.3	151.2	1165.1	3044.4
258.7	1353.1	3111.9	128.1	1177.0	3051.5	120.9	1285.3	3093.4	161.7	1199.7	3044.7
259.1	1389.0	3113.6	143.0	1181.7	3054.3	150.1	1286.3	3108.9	172.1	1210.8	3045.7
274.3	1392.2	3114.8	154.5	1192.1	3058.0	166.3	1287.8	3110.5	187.5	1219.5	3067.8
319.5	1394.8	3117.9	184.7	1279.5	3067.7	168.2	1389.2	3113.2	215.3	1279.1	3084.1
353.1	1395.8	3118.6	255.8	1281.6	3078.2	175.5	1389.9	3116.7	223.4	1287.8	3087.8
365.7	1399.3	3118.9	258.6	1283.7	3080.9	257.4	1393.3	3118.2	258.6	1299.1	3089.3
392.6	1400.2	3364.3	258.9	1285.2	3085.3	258.7	1396.5	3120.2	270.9	1302.3	3091.3
412.9	1413.4	3373.0	270.3	1350.8	3092.7	260.5	1397.9	3120.7	272.4	1348.5	3108.5
438.9	1424.2	3417.1	330.7	1372.6	3109.4	261.2	1399.9	3120.9	277.3	1358.9	3109.5
450.9	1426.3	3433.6	361.7	1391.1	3114.5	410.0	1401.6	3324.6	346.8	1394.8	3110.4
467.7	1427.1	3437.5	366.3	1394.2	3115.4	424.2	1403.8	3373.6	367.5	1395.5	3117.4
490.0	1439.7	3465.2	394.5	3543.7	3116.4	431.8	1424.9	3461.9	399.2	1396.6	3117.4
503.3	1497.0	3525.9	409.1	1394.7	3118.4	437.0	1425.4	3476.4	409.1	1398.4	3118.6
523.2	1497.7	3547.2	430.6	1396.6	3118.7	447.1	1427.2	3486.1	427.5	1414.3	3124.4
784.5	1497.9		449.0	1398.8	3119.0	454.4	1427.6	3488.9	447.3	1416.3	3124.6
789.1	1498.0		467.7	1400.1	3119.7	459.0	1495.6	3546.6	495.6	1420.1	3266.2
790.5	1499.3		489.8	1415.8	3370.2	486.7	1497.3	3557.2	526.1	1425.9	3308.5
811.3	1500.9		508.0	1424.2	3406.8	784.3	1498.3		536.9	1426.8	3339.8
900.9	1501.5		517.1	1426.7	3426.5	790.0	1499.1		552.4	1427.5	3507.1
902.5	1508.7		534.7	1427.7	3458.6	791.0	1499.6		618.7	1453.3	3534.0
903.0	1513.1		544.9	1441.8	3461.6	793.3	1499.8		746.0	1498.4	3534.4
903.8	1515.8		783.0	1496.9	3479.1	901.3	1501.9		791.3	1499.1	3536.3
977.5	1517.9		790.8	1497.4	3541.8	902.6	1502.1		798.4	1499.4	3575.3
H_2r1			CHTS1			CHp1			OHTS1		
17.0	746.1	1499.5	-467.6	799.0	1499.6	11.8	798.4	1499.4	-1375.4	798.9	1499.7
20.0	1498.5	1500.2	13.9	800.7	1499.7	16.4	800.6	1499.8	15.2	814.2	1499.9
26.0	790.9	1502.6	15.2	814.0	1500.4	27.2	813.6	1502.6	21.0	820.2	1501.2
31.1	799.5	1503.0	27.7	902.3	1502.7	28.4	902.1	1502.7	23.8	902.9	1502.9
33.2	801.3	1504.0	30.8	904.8	1503.0	31.7	904.9	1503.2	29.5	904.9	1503.4
43.7	813.3	1505.7	35.1	907.5	1503.5	37.5	907.6	1504.8	33.7	906.8	1504.9
48.3	902.5	1517.3	43.8	908.0	1505.4	45.4	908.2	1516.7	36.3	907.5	1516.8
49.6	904.7	1517.6	48.5	962.0	1517.0	50.8	958.1	1517.2	42.7	967.3	1518.1
52.9	907.2	1519.1	53.1	1013.5	1517.6	53.6	1015.3	1518.7	48.5	1006.9	1519.1
58.4	908.0	1537.6	54.1	1018.9	1519.3	61.7	1019.0	1537.5	52.7	1020.7	1537.1
61.9	964.0	1661.9	62.3	1028.6	1537.3	66.0	1030.1	1653.4	57.5	1026.5	1661.2
70.1	1014.3	1674.5	69.0	1029.8	1661.7	67.3	1031.5	1661.2	62.9	1029.5	1669.2
71.2	1020.2	1691.5	76.2	1057.1	1677.7	71.4	1061.8	1681.7	69.8	1044.6	1685.1
77.3	1028.4	1693.7	84.0	1082.8	1695.5	81.2	1086.2	1700.5	82.3	1063.5	1697.6
84.6	1029.8	1711.8	91.1	1084.7	1699.3	89.2	1086.4	1704.4	89.6	1081.9	1732.0
88.1	1055.8	3024.8	94.1	1088.2	1706.4	93.8	1087.7	2896.4	91.9	1087.8	3024.7
91.7	1081.6	3039.3	99.9	1092.3	3023.6	105.2	1089.0	3018.5	99.2	1090.0	3029.8
100.2	1084.2	3041.9	112.9	1100.9	3038.5	111.9	1096.4	3032.9	107.8	1091.6	3041.1
105.1	1088.0	3043.8	131.3	1109.1	3043.1	118.3	1106.2	3040.4	114.7	1095.6	3045.1
113.7	1090.9	3044.3	137.2	1120.2	3043.4	128.8	1122.4	3042.3	131.1	1116.6	3045.3
130.4	1098.9	3044.9	160.1	1165.3	3044.5	132.9	1164.5	3042.6	152.9	1166.4	3046.0
131.0	1119.6	3046.3	172.3	1200.6	3045.2	154.5	1204.3	3043.7	157.0	1191.2	3046.3
152.0	1166.1	3067.6	187.8	1215.9	3045.8	162.6	1222.3	3045.3	184.1	1206.3	3047.4
161.9	1200.2	3081.9	199.3	1221.0	3068.2	178.2	1227.8	3066.1	188.5	1217.1	3068.5
172.0	1212.9	3087.7	224.2	1279.1	3082.9	188.8	1278.8	3080.2	206.6	1280.7	3077.5
187.4	1220.5	3089.8	258.4	1288.9	3085.2	224.0	1290.9	3084.0	258.5	1284.6	3079.0

215.3	1279.8	3091.5	269.1	1300.4	3089.8	235.0	1303.2	3089.6	261.9	1291.4	3089.2
219.3	1287.3	3108.3	270.9	1303.5	3091.6	258.4	1306.5	3089.8	268.9	1300.1	3092.6
223.8	1299.4	3109.3	278.0	1335.6	3108.1	271.1	1360.7	3105.3	274.4	1325.5	3109.1
259.5	1302.5	3110.8	295.0	1359.8	3109.5	273.4	1390.1	3107.6	325.7	1357.9	3110.8
270.8	1348.6	3117.0	345.5	1387.2	3110.7	283.3	1394.4	3110.4	346.5	1394.9	3111.6
271.6	1358.4	3118.2	368.5	1395.1	3117.6	347.1	1395.5	3116.2	357.1	1396.0	3118.3
277.3	1394.8	3119.3	374.1	1395.6	3117.6	370.3	1396.0	3116.8	389.4	1398.4	3118.8
351.7	1395.8	3124.6	400.4	1396.5	3119.0	402.3	1398.6	3117.2	403.0	1399.1	3121.0
368.6	1396.7	3124.8	411.1	1398.7	3124.2	411.0	1405.7	3123.4	430.4	1405.4	3123.3
399.6	1398.6	3263.0	428.5	1414.4	3124.8	429.4	1413.9	3124.6	453.9	1411.7	3125.9
409.0	1414.7	3309.3	448.4	1418.4	3248.6	448.1	1419.4	3191.0	489.5	1415.6	3302.8
430.2	1416.8	3340.7	495.7	1420.3	3300.7	495.8	1423.2	3251.3	502.6	1420.6	3418.6
447.8	1420.4	3508.4	525.3	1426.1	3338.7	529.9	1426.5	3300.8	522.5	1426.9	3432.2
494.4	1425.9	3533.8	541.0	1426.9	3506.9	547.6	1426.9	3508.1	552.2	1428.1	3504.5
525.9	1426.7	3534.4	559.0	1427.8	3533.4	568.5	1428.0	3529.7	602.9	1429.6	3531.5
536.9	1427.2	3535.8	623.8	1453.4	3535.7	627.7	1455.1	3535.0	677.5	1451.6	3534.9
552.6	1453.5	3576.4	781.4	1498.3	3536.7	769.5	1498.2	3536.0	792.2	1498.1	3539.5
618.9	1499.2	4398.9	791.3	1499.2	3574.8	791.1	1498.6	3576.5	795.7	1498.7	3571.9
OHp1			eTS2			rFA			H_2r2		
12.2	816.8	1500.1	-775.0	795.1	1498.8	18.0	808.0	1499.0	14.9	792.8	1497.9
19.1	902.7	1500.3	19.1	816.0	1501.0	21.1	851.5	1499.2	17.2	795.5	1498.8
29.4	903.9	1502.6	25.1	902.0	1502.8	24.1	902.5	1501.1	27.5	799.3	1499.2
31.2	905.7	1503.7	29.3	903.8	1503.4	28.7	905.5	1501.3	30.5	827.7	1501.3
37.8	906.9	1508.3	34.5	904.2	1505.5	29.9	905.7	1502.4	35.3	845.0	1501.8
42.7	964.9	1515.2	41.7	906.9	1513.9	37.0	907.8	1503.1	38.7	902.2	1502.6
46.4	1010.8	1517.7	43.7	969.7	1514.9	42.4	953.1	1515.1	44.1	905.1	1513.4
49.2	1017.6	1518.9	51.4	994.1	1518.8	47.8	984.5	1516.6	48.4	907.9	1514.8
57.3	1021.8	1534.5	57.8	1009.8	1535.0	52.5	1017.0	1519.0	52.7	911.0	1518.4
59.3	1025.6	1633.6	58.1	1019.7	1633.6	59.8	1017.5	1533.6	57.0	953.9	1518.9
62.4	1031.3	1651.6	64.6	1026.6	1651.5	61.6	1021.0	1661.1	68.0	980.4	1533.8
69.6	1044.1	1662.4	66.9	1029.1	1661.7	72.9	1031.6	1681.9	71.6	1015.3	1660.2
71.9	1056.9	1679.5	75.4	1043.6	1676.5	79.7	1064.4	1689.9	76.4	1020.6	1686.2
82.5	1061.2	1802.9	76.8	1048.7	1689.4	82.9	1073.8	1704.9	81.7	1026.5	1697.4
87.8	1087.3	2930.9	88.3	1066.9	3025.9	87.6	1086.7	2898.4	83.9	1031.4	1706.8
91.9	1088.5	3032.3	90.5	1085.5	3041.2	96.7	1089.0	3016.0	89.2	1067.3	2903.7
105.1	1092.6	3045.5	95.4	1087.8	3041.8	113.2	1092.2	3037.1	96.7	1086.4	3010.8
119.1	1109.7	3045.8	102.9	1091.2	3044.6	123.5	1103.5	3039.0	101.8	1088.2	3030.8
124.9	1164.0	3045.9	124.3	1115.9	3045.9	143.6	1127.6	3041.4	109.6	1092.8	3040.5
126.1	1167.1	3046.8	133.0	1167.8	3046.6	160.0	1142.8	3043.6	115.9	1096.7	3042.1
137.6	1187.9	3047.3	149.4	1191.3	3048.8	180.0	1164.1	3045.0	126.3	1113.3	3044.0
160.1	1198.5	3051.2	160.2	1192.6	3070.6	185.4	1199.6	3045.1	154.3	1118.6	3044.7
177.4	1205.8	3061.8	173.5	1209.7	3079.3	213.1	1208.4	3067.1	167.3	1150.3	3045.8
185.2	1267.7	3066.1	189.8	1231.4	3084.1	237.5	1231.4	3071.0	178.2	1163.8	3050.5
258.9	1278.5	3073.5	223.5	1280.4	3093.0	258.3	1278.4	3080.7	183.5	1201.6	3069.5
262.0	1280.7	3080.6	258.5	1283.1	3093.4	260.5	1294.1	3083.3	219.5	1206.2	3076.1
269.4	1287.0	3089.1	263.2	1286.3	3105.9	271.0	1295.9	3090.6	247.1	1214.6	3087.6
274.1	1293.5	3090.6	271.3	1292.8	3110.4	276.3	1303.1	3102.0	258.7	1280.2	3092.0
340.4	1347.6	3108.9	273.3	1353.9	3110.8	277.8	1310.4	3105.4	265.4	1294.3	3107.1
346.8	1390.6	3111.0	348.1	1380.9	3113.7	339.6	1365.3	3108.1	277.8	1298.1	3109.3
383.7	1394.6	3111.8	364.6	1390.9	3117.9	360.4	1392.6	3108.2	290.8	1303.5	3113.2
397.8	1397.8	3117.3	386.6	1396.6	3119.1	405.3	1394.1	3114.5	324.1	1310.8	3116.2
439.0	1398.4	3117.6	392.3	1397.8	3120.9	413.0	1397.1	3115.9	337.8	1363.6	3117.7
443.9	1399.5	3117.9	420.5	1399.2	3126.0	428.2	1398.5	3116.8	349.8	1391.6	3121.3
457.3	1410.0	3121.2	442.7	1403.2	3126.9	445.6	1411.5	3122.5	375.7	1396.5	3124.2
481.8	1414.6	3126.3	466.1	1409.6	3270.1	486.8	1412.4	3123.4	381.2	1397.8	3124.8
512.6	1415.4	3322.5	502.7	1417.3	3326.1	520.8	1416.4	3203.8	393.8	1399.5	3139.0
537.9	1426.9	3372.9	516.9	1425.8	3404.0	534.7	1422.9	3375.4	429.3	1409.9	3189.5
556.2	1427.0	3432.5	531.9	1426.0	3424.4	558.6	1423.8	3509.7	441.1	1414.9	3367.8
595.6	1427.9	3486.6	545.0	1428.0	3478.0	567.1	1426.6	3537.9	452.1	1417.0	3507.7
701.2	1444.9	3500.8	599.4	1452.1	3497.2	631.4	1453.3	3538.8	485.1	1423.1	3539.4
791.5	1497.1	3521.4	665.5	1495.5	3532.9	790.1	1472.1	3539.3	501.1	1425.9	3541.0
792.5	1499.0	3533.6	786.6	1495.9	3538.6	794.6	1497.1	3578.4	532.7	1426.9	3548.7
796.7	1499.4	3568.9	792.5	1496.6	3565.4	796.4	1498.7	3864.8	560.1	1447.2	3577.7
									579.1	1474.8	3846.0
									623.5	1497.0	4356.1
CHTS2			CHp2			OHTS2			OHp2		
-435.0	849.6	1508.8	15.1	811.1	1499.3	-504.8	795.5	1499.0	17.5	900.8	1499.8
51.6	852.8	1510.2	25.4	813.4	1501.2	6.5	809.2	1499.4	23.0	903.0	1500.9
59.7	879.5	1510.4	31.2	901.3	1502.0	21.6	889.8	1500.5	26.9	905.4	1502.4
71.6	896.5	1512.6	41.5	902.9	1502.9	26.9	902.6	1501.3	31.6	906.0	1502.8
82.1	901.6	1513.0	42.8	906.6	1503.4	33.6	905.8	1502.5	32.9	965.5	1508.6
83.3	905.5	1515.1	45.4	908.4	1507.6	34.8	906.2	1504.6	39.1	1006.5	1516.5
91.1	906.6	1523.1	48.4	909.4	1518.2	38.0	908.3	1516.8	42.3	1015.0	1517.3
108.0	1030.5	1527.9	55.7	958.6	1520.5	42.8	955.6	1517.4	43.1	1018.5	1519.4
112.8	1042.7	1531.5	58.0	1015.1	1525.9	53.5	1014.4	1518.2	49.0	1021.6	1519.8
118.1	1056.6	1533.3	71.6	1021.3	1527.5	55.5	1018.8	1531.6	58.1	1032.5	1530.0
120.6	1057.0	1545.1	75.6	1030.5	1536.6	62.2	1023.0	1534.9	62.2	1034.9	1624.0
130.8	1058.1	1677.4	77.4	1032.2	1661.3	68.9	1035.2	1662.4	71.1	1044.2	1663.2
137.2	1059.7	1701.6	79.7	1038.2	1693.4	75.5	1052.3	1669.8	75.3	1052.3	1681.3

141.1	1071.4	1709.6	89.6	1057.1	1703.4	76.7	1058.6	1686.6	81.4	1065.8	1692.8
156.5	1076.6	1720.6	101.3	1073.3	1718.3	82.5	1083.8	1698.9	88.1	1084.6	3034.5
170.8	1096.6	1836.0	110.4	1085.7	2940.9	89.5	1088.3	2920.8	93.5	1087.6	3043.0
184.6	1098.8	2765.5	116.1	1087.7	2964.4	100.6	1091.6	2938.5	101.0	1088.4	3043.5
191.4	1118.6	2899.4	128.0	1100.4	3016.0	107.5	1098.3	3021.4	120.0	1092.9	3045.0
202.7	1132.7	2914.1	134.5	1119.0	3025.8	125.2	1108.9	3040.2	133.8	1110.3	3046.6
214.7	1147.4	2926.2	157.4	1128.0	3029.9	128.3	1124.0	3040.9	143.9	1166.8	3047.9
219.4	1155.2	2934.7	173.6	1164.6	3036.6	144.9	1155.0	3042.2	148.5	1192.7	3050.4
236.1	1188.1	2937.1	180.1	1194.9	3043.6	159.6	1164.2	3045.1	175.5	1195.7	3053.5
245.0	1241.9	2939.2	191.3	1201.8	3044.3	168.0	1192.9	3045.3	185.7	1200.1	3065.9
272.9	1243.3	2940.1	200.7	1217.6	3044.9	172.7	1206.5	3046.0	190.7	1212.6	3070.8
305.5	1251.0	2940.3	232.6	1233.8	3072.3	185.7	1222.5	3066.4	258.9	1279.3	3082.9
335.7	1272.2	2946.3	258.3	1253.3	3073.4	224.1	1272.2	3068.5	265.1	1280.8	3086.1
370.1	1297.8	2961.0	266.4	1280.3	3074.8	258.6	1278.6	3074.6	270.0	1290.3	3090.4
400.2	1311.7	2962.3	282.3	1290.6	3086.9	263.9	1282.3	3086.0	278.8	1294.3	3107.5
400.7	1315.1	2980.0	284.7	1294.7	3094.4	266.0	1290.0	3091.9	341.0	1356.2	3110.9
404.7	1315.2	2980.5	342.7	1302.9	3101.2	271.3	1292.4	3107.1	354.4	1393.8	3111.5
408.5	1325.4	2997.5	364.3	1353.0	3102.4	331.6	1299.0	3107.9	378.9	1394.6	3112.1
410.9	1394.5	2999.9	376.8	1357.1	3107.9	343.6	1359.1	3109.2	406.5	1396.2	3117.4
416.5	1401.4	3002.9	404.8	1359.8	3110.4	368.7	1393.9	3114.3	437.7	1397.6	3117.6
431.0	1413.1	3005.6	413.9	1391.9	3116.8	385.6	1395.2	3116.3	446.5	1398.9	3122.6
462.3	1414.4	3006.2	426.1	1398.3	3117.1	410.9	1397.4	3117.7	448.7	1402.1	3122.7
463.1	1416.4	3006.9	447.7	1400.2	3118.0	433.8	1398.7	3122.3	481.4	1411.5	3139.6
496.7	1418.3	3015.2	459.5	1412.7	3120.1	441.3	1406.4	3122.6	488.9	1412.1	3282.5
500.2	1430.1	3016.4	477.4	1413.9	3121.1	479.6	1410.8	3266.0	494.1	1423.2	3398.0
507.2	1434.3	3019.3	500.4	1416.2	3225.6	518.9	1413.3	3327.3	515.0	1426.0	3423.7
546.7	1436.5	3250.1	510.7	1423.4	3346.2	524.7	1423.3	3410.0	551.9	1427.1	3456.5
555.0	1441.2	3380.4	548.9	1426.2	3505.9	536.6	1424.5	3507.4	567.0	1427.8	3491.8
630.5	1443.7	3402.9	580.5	1427.2	3528.1	563.6	1426.9	3534.7	580.8	1438.5	3501.6
667.7	1445.9	3410.8	590.5	1449.7	3529.7	597.0	1443.0	3536.0	791.9	1441.7	3502.4
702.7	1459.1	3413.1	631.9	1453.6	3534.7	607.5	1449.2	3543.5	795.1	1498.1	3534.9
808.6	1473.7	3439.2	792.7	1497.1	3575.2	790.2	1497.5	3576.1	795.2	1499.2	3565.0
848.9	1505.9	3695.9	800.4	1497.7	3836.6	795.3	1498.7	3842.6	810.6	1499.4	3570.8

Table S11. Harmonic vibrational frequencies (cm^{-1}) for the reactants, products, and intermediates of the $Li(H_2O)_4 + CO_2 + 2H_2 \rightarrow Li(H_2O)_4 + CH_2(OH)_2$ reaction pathway.

$Li(H_2O)_4$			CO_2r			eTS1			CO_2p		
56.4	376.2	3698.4	15.8	251.8	1396.7	-544.7	228.6	1275.2	25.8	340.6	1368.3
60.2	392.2	3743.8	28.1	274.1	1566.7	17.5	253.3	1583.0	41.9	342.3	1593.6
78.8	413.5	3750.1	53.5	363.0	1586.3	34.8	274.4	1588.2	60.0	367.9	1596.7
80.3	452.2	3864.1	56.5	368.5	1598.9	46.3	321.2	1609.4	91.3	396.4	1677.3
116.0	460.1	3865.4	66.4	379.6	1630.0	55.3	332.5	1613.9	101.4	437.4	1684.6
125.0	499.9		79.7	395.9	2444.6	73.8	364.0	2320.8	117.4	453.1	1715.5
143.0	574.7		97.5	425.2	3518.5	78.2	364.8	3571.2	130.3	498.1	2702.6
197.0	1557.7		103.9	442.7	3543.3	93.8	385.1	3617.5	149.1	534.0	2815.3
197.3	1580.7		109.6	480.3	3597.6	96.9	412.3	3646.6	197.5	621.8	3755.7
254.1	1599.5		126.9	486.6	3661.4	118.6	446.1	3675.9	219.7	652.0	3756.1
271.0	1602.9		148.9	532.4	3751.5	143.2	476.0	3731.0	225.2	658.3	3904.1
316.9	3465.5		161.7	562.9	3757.3	156.9	500.4	3766.9	254.3	742.2	3904.7
327.1	3471.5		193.4	655.9	3776.3	173.0	543.4	3830.8	285.8	1022.0	3925.1
371.1	3686.1		219.8	668.6	3895.7	208.4	587.8	3879.6	302.4	1048.7	3925.4
H_2r1			CHTS1			CHp1			OHTS1		
12.8	299.4	1039.2	-1160.3	344.8	1227.6	20.7	319.2	1408.2	-1055.8	330.9	1324.9
24.4	337.1	1367.7	27.0	353.2	1290.2	24.2	352.6	1419.5	44.8	336.2	1417.3
27.7	339.7	1594.0	42.7	380.0	1449.7	34.0	361.3	1585.8	61.5	401.1	1596.8
43.3	349.4	1596.9	61.6	397.2	1592.7	43.3	383.4	1595.7	82.9	432.9	1609.1
60.0	365.0	1677.8	91.9	417.0	1595.9	64.0	410.5	1629.6	90.0	458.7	1656.5
90.7	388.2	1685.4	101.5	443.0	1685.7	93.3	458.6	1699.9	97.1	485.4	1688.6
100.2	393.4	1717.0	106.0	455.5	1697.1	107.9	459.1	1707.3	126.5	526.9	1730.1
115.2	437.6	2741.7	116.7	502.6	1711.8	112.5	532.7	2387.1	130.2	561.9	3047.1
130.1	453.5	2849.4	132.9	538.2	2669.1	124.4	580.9	2507.6	152.7	591.6	3115.8
144.8	492.4	3761.3	147.9	626.7	2766.7	138.4	645.9	2949.3	164.6	619.1	3221.7
174.4	526.5	3763.2	196.0	658.1	3755.5	165.0	693.5	3712.8	188.4	663.7	3519.8
193.9	619.1	3903.6	218.7	664.8	3755.6	204.0	696.9	3713.4	202.9	713.8	3793.5
216.0	646.6	3904.2	253.7	747.6	3906.9	218.1	772.6	3910.8	221.5	766.2	3857.5
225.4	653.6	3925.9	257.9	1045.1	3906.9	237.6	1083.0	3910.9	252.2	909.7	3874.2
253.3	742.2	3926.5	304.5	1067.4	3925.8	256.8	1125.8	3922.3	266.2	940.3	3884.5
284.1	1011.5	4357.5	308.6	1113.7	3926.2	288.3	1144.5	3922.7	313.4	1082.1	3931.9
OHp1			eTS2			rFA			H_2r2		
16.1	350.6	1593.5	-550.8	336.1	1609.5	40.5	364.6	1618.5	11.7	306.1	1176.1
38.6	382.9	1608.4	-191.6	394.5	1656.3	75.9	378.8	1646.6	27.9	323.1	1309.0
49.8	410.3	1641.8	-143.1	432.9	1695.9	84.3	462.1	1652.4	38.6	335.6	1420.3
65.0	412.4	1882.1	-102.2	481.0	1751.5	96.5	496.7	1697.1	45.3	349.3	1612.4
75.3	440.0	3025.8	82.3	502.0	2927.3	104.2	536.6	2749.9	62.7	356.2	1648.8
90.4	474.3	3282.5	92.2	537.2	3107.4	110.4	578.4	2955.1	92.9	389.8	1663.1
107.4	500.9	3381.9	107.2	575.1	3127.9	125.8	613.3	3003.4	112.5	453.8	1715.2
114.6	537.5	3455.1	121.6	615.9	3212.4	159.9	628.2	3191.8	122.5	503.1	2884.5
118.1	571.2	3580.4	141.8	628.1	3707.5	215.1	663.7	3738.9	132.3	533.2	2984.1
130.0	611.5	3649.2	165.2	638.6	3756.7	231.2	802.6	3869.6	139.3	571.3	3113.1
176.0	732.8	3698.6	184.5	697.7	3833.3	245.3	940.5	3885.2	141.7	582.0	3238.1
196.0	870.1	3792.2	195.6	860.5	3902.6	253.8	982.0	3903.6	226.4	639.5	3728.7
215.7	1055.1	3802.3	233.8	986.5	3908.6	282.1	1048.9	3907.4	237.4	673.9	3872.8
233.1	1165.5	3906.9	251.4	1042.9	3909.0	287.5	1062.1	3922.6	248.3	872.0	3898.6
243.2	1346.4		261.6	1292.2		308.4	1195.1		255.3	905.6	3907.6
298.6	1421.4		290.9	1400.3		325.6	1318.3		285.0	937.8	3912.9
315.8	1525.3		309.8	1573.9		340.2	1446.0		296.1	1022.9	3915.3
									301.0	1061.0	4348.4
CHTS2			CHp2			OHTS2			OHp2		
-782.0	355.0	1287.9	37.1	362.0	1375.1	-192.0	355.2	1282.8	38.4	386.1	1443.4
-37.0	380.3	1345.1	47.7	364.3	1442.5	52.2	413.8	1435.7	49.4	409.4	1520.3
54.7	414.3	1400.7	63.8	375.0	1535.7	67.8	445.8	1534.2	58.8	430.0	1546.8
66.4	416.1	1459.9	95.6	395.9	1611.3	86.1	469.7	1593.5	77.6	457.5	1606.8
80.6	446.0	1627.5	104.5	455.6	1640.2	116.3	510.7	1620.3	89.8	481.8	1634.7

101.4	471.3	1662.9	129.2	498.6	1656.4	118.4	516.6	1694.1	106.4	524.3	1657.4
119.2	527.4	1684.7	136.5	537.4	1710.4	144.8	555.5	1717.4	116.1	528.5	3086.3
133.3	567.9	1731.4	141.8	578.0	2839.3	147.6	597.5	2928.2	127.7	548.0	3144.3
142.4	572.4	2875.2	188.2	596.8	2968.8	172.1	625.1	2969.0	137.8	562.8	3289.1
211.4	635.2	2955.5	193.0	617.9	3002.3	187.8	635.3	2989.2	177.9	598.2	3383.2
226.7	672.5	3107.2	237.7	670.9	3024.1	199.3	664.0	3458.6	192.9	714.2	3481.4
232.4	873.5	3320.0	241.5	881.3	3240.4	212.5	747.4	3582.1	225.9	824.3	3581.4
241.7	902.6	3738.4	257.1	974.3	3741.9	245.8	845.1	3680.2	250.1	1015.0	3630.3
263.1	1000.3	3806.5	288.5	1022.5	3828.5	264.5	868.9	3736.9	253.1	1044.0	3703.2
299.0	1043.1	3872.9	297.8	1038.4	3902.8	290.4	972.1	3851.2	307.3	1076.8	3746.7
334.2	1116.8	3893.3	316.3	1089.1	3907.5	314.2	1109.5	3908.7	320.9	1205.8	3830.9
343.8	1174.0	3893.9	332.8	1158.0	3908.3	335.3	1154.1	3912.8	342.3	1389.1	3880.1
351.3	1233.1	3897.2	341.4	1269.3	3912.9	343.2	1271.6	3929.8	369.3	1399.5	3890.3

Table S12. Harmonic vibrational frequencies (cm^{-1}) for the reactants, products, and intermediates of the $Li(CH_3OH)_4 + CO_2 + 2H_2 \rightarrow Li(CH_3OH)_4 + CH_2(OH)_2$ reaction pathway.

$Li(CH_3OH)_4$			CO_2r			eTS1			CO_2p		
28.5	1061.0	1517.5	-29.5	498.7	1490.3	-421.1	501.6	1505.0	24.9	493.5	1501.1
30.4	1064.1	3042.2	13.4	531.7	1497.6	48.2	510.6	1509.0	28.0	526.3	1503.1
35.6	1070.4	3044.2	24.0	543.4	1498.7	51.7	569.9	1509.4	32.3	727.5	1504.6
52.0	1093.8	3045.3	30.3	550.8	1506.6	60.3	638.4	1516.0	48.3	799.4	1505.7
53.9	1104.1	3051.4	34.4	583.6	1507.1	71.5	650.9	1516.0	59.2	839.4	1515.0
73.8	1106.7	3103.8	39.6	585.8	1515.7	75.0	667.7	1525.3	64.1	910.9	1517.6
83.3	1107.8	3107.4	42.6	1050.2	1516.4	92.0	1043.9	1526.2	75.7	1062.8	1524.9
87.0	1182.3	3109.2	49.3	1064.0	1519.1	100.3	1057.7	1527.8	78.4	1083.7	1529.2
90.1	1182.7	3114.7	56.2	1082.5	1521.0	103.0	1076.4	1528.4	85.8	1094.7	1536.2
93.6	1183.1	3137.6	63.5	1087.7	2421.7	114.8	1083.6	2297.5	90.5	1096.3	1710.7
98.7	1186.9	3138.3	69.1	1097.8	3043.0	123.2	1130.6	2960.8	98.8	1104.8	3034.1
114.9	1374.9	3138.6	73.3	1100.7	3043.1	127.6	1133.2	2962.0	104.2	1152.2	3035.6
129.4	1377.1	3163.3	96.0	1110.9	3046.2	135.0	1144.4	2962.5	104.5	1159.8	3042.2
138.6	1380.4	3325.8	96.8	1120.3	3047.5	150.6	1151.8	2963.7	119.6	1162.4	3051.2
157.6	1383.8	3333.0	104.1	1178.5	3104.5	154.8	1204.2	3016.7	126.9	1187.9	3092.2
182.8	1475.2	3408.7	106.8	1179.4	3105.9	168.3	1204.4	3019.9	138.3	1191.1	3095.0
191.9	1476.7	3876.9	112.2	1188.3	3107.7	184.6	1209.0	3021.8	146.2	1191.1	3104.6
242.3	1476.9		128.7	1189.0	3108.7	220.9	1209.6	3025.5	168.7	1193.7	3114.0
295.9	1489.5		137.0	1360.2	3139.7	242.7	1267.0	3042.5	183.8	1353.7	3117.3
447.2	1498.9		152.4	1369.4	3141.8	255.5	1382.7	3050.5	190.2	1376.2	3127.6
451.3	1500.1		190.4	1373.1	3147.0	300.5	1399.3	3058.3	239.5	1459.5	3128.9
463.4	1500.5		216.2	1380.4	3148.6	302.6	1400.7	3060.7	241.1	1481.0	3166.1
495.9	1513.3		234.4	1406.0	3236.4	304.1	1423.8	3061.1	280.8	1488.0	3223.1
525.9	1516.2		322.1	1470.5	3253.9	305.7	1486.9	3066.0	297.1	1490.3	3367.3
560.6	1516.4		389.0	1473.7	3752.4	382.1	1490.1	3644.2	298.5	1491.3	3444.4
1058.5	1517.0		467.8	1489.6	3761.9	489.6	1504.0	3650.5	443.2	1493.7	3888.6
H_2r1			CHTS1			CHp1			OHTS1		
21.6	344.3	1493.2	-1160.4	439.8	1491.4	25.8	437.9	1499.4	-801.6	499.9	1489.9
23.7	360.5	1500.4	23.9	493.5	1495.1	30.2	499.7	1502.9	26.3	569.1	1491.3
24.6	441.5	1503.2	26.9	530.5	1503.2	35.7	527.4	1504.3	27.7	678.8	1498.8
27.9	493.8	1504.4	32.6	730.1	1503.6	40.5	752.5	1505.2	39.4	721.4	1504.1
31.8	526.8	1505.6	48.1	809.3	1505.4	50.9	843.0	1512.6	45.0	802.7	1505.8
48.2	726.5	1514.9	58.7	845.7	1508.2	55.1	886.8	1515.0	62.8	865.4	1515.7
58.6	791.8	1517.6	61.1	929.5	1515.2	61.9	988.1	1517.8	66.7	960.2	1517.4
63.8	831.6	1524.6	67.3	1062.4	1517.6	78.4	1065.1	1528.2	72.9	1063.8	1519.8
75.2	904.6	1528.3	77.1	1084.5	1524.8	82.7	1087.3	1533.1	81.0	1066.1	1523.2
77.5	1062.5	1535.3	83.5	1094.7	1530.6	86.0	1093.4	1568.8	86.8	1079.2	1527.5
85.3	1082.8	1713.0	87.9	1097.9	1544.7	87.2	1093.6	1657.6	91.0	1088.8	1740.4
89.7	1094.6	3034.7	91.7	1105.4	1711.1	95.1	1095.0	2964.5	96.1	1093.0	3038.5
97.7	1095.9	3036.6	98.6	1126.7	3032.1	97.2	1112.5	3005.6	99.9	1098.8	3041.0
102.6	1104.0	3043.0	103.4	1152.3	3035.5	100.5	1154.8	3036.9	103.7	1130.2	3042.3
103.3	1151.3	3051.5	106.3	1161.9	3041.7	107.2	1164.4	3037.7	107.9	1146.1	3049.8
118.7	1159.0	3093.7	124.1	1164.8	3051.4	112.1	1172.2	3049.7	119.4	1152.9	3057.3
126.0	1161.6	3095.6	134.4	1187.9	3092.3	121.5	1187.4	3051.5	125.6	1185.7	3096.7
137.0	1187.8	3105.5	141.6	1191.1	3093.1	144.8	1191.6	3081.8	137.0	1188.1	3100.5
144.6	1190.9	3114.4	148.1	1191.1	3103.7	147.1	1192.2	3096.4	155.0	1191.1	3106.2
164.2	1190.9	3118.1	169.4	1193.3	3114.3	171.5	1192.5	3096.8	157.5	1191.8	3111.4
167.4	1193.4	3128.5	180.3	1220.5	3116.0	184.0	1375.6	3110.2	172.6	1324.9	3127.4
183.6	1351.4	3129.9	238.0	1293.6	3127.7	187.7	1381.0	3112.2	197.4	1375.8	3131.1
192.1	1376.3	3166.2	240.6	1376.3	3128.5	196.2	1414.2	3122.0	232.1	1411.3	3133.2
236.8	1458.0	3236.7	254.4	1430.3	3166.0	235.9	1483.0	3124.8	248.9	1421.3	3166.0
240.4	1478.9	3384.7	295.1	1462.3	3192.1	247.7	1485.4	3161.9	275.5	1456.4	3186.2
279.4	1488.0	3456.5	300.1	1485.7	3364.6	291.4	1487.9	3304.0	311.6	1478.5	3404.3
294.5	1490.2	3888.3	344.3	1488.9	3441.8	297.4	1490.8	3386.1	426.3	1482.0	3549.5
297.6	1491.3	4362.4	405.8	1490.8	3888.4	320.9	1492.6	3888.4	487.4	1489.0	3883.2
OHp1			eTS2			rFA			H_2r2		

13.4	525.9	1492.6	-352.3	495.1	1492.6	25.1	525.5	1501.8	23.1	410.7	1491.7
27.1	567.8	1498.5	21.4	511.2	1501.1	33.0	558.6	1504.2	27.3	465.9	1501.6
33.3	651.4	1500.0	28.5	542.5	1503.6	41.2	860.5	1504.9	32.7	469.5	1504.1
33.8	700.2	1507.8	33.6	638.9	1505.5	46.6	896.2	1508.1	40.5	527.2	1504.9
46.8	861.6	1508.0	38.7	668.8	1514.4	56.1	954.2	1516.1	44.6	559.9	1507.8
59.9	1067.0	1518.2	47.8	894.7	1516.5	63.5	971.6	1516.5	48.3	863.4	1515.9
72.6	1070.2	1518.5	55.8	1045.5	1518.7	76.6	1031.0	1517.3	58.5	895.7	1516.4
78.0	1071.8	1519.1	59.0	1061.1	1521.5	90.7	1066.1	1525.8	63.3	950.8	1517.1
82.7	1079.2	1527.7	74.2	1066.4	1528.3	91.8	1084.9	1536.0	77.1	971.3	1525.4
86.2	1090.0	1785.4	80.8	1075.5	1664.2	93.9	1094.0	1570.5	91.0	1020.9	1535.6
92.3	1094.1	2912.6	85.8	1093.8	3034.5	95.9	1108.8	2909.1	93.0	1065.7	1566.6
100.0	1109.1	3042.2	91.9	1094.4	3041.1	105.3	1117.0	2970.4	93.7	1084.4	2935.4
102.3	1121.8	3042.9	96.8	1111.3	3050.8	111.3	1140.1	3017.8	96.1	1094.0	2975.5
106.0	1148.1	3044.1	107.8	1120.2	3051.8	114.0	1167.5	3030.3	103.8	1107.8	3021.8
118.1	1183.7	3046.6	109.7	1156.9	3094.9	131.1	1169.7	3037.3	110.8	1115.9	3033.2
123.8	1184.1	3073.6	119.4	1182.6	3101.3	132.8	1182.3	3048.3	116.8	1141.0	3038.0
128.8	1185.1	3103.5	131.9	1188.0	3112.8	147.7	1188.5	3076.2	130.9	1166.7	3049.0
153.4	1189.2	3104.3	137.8	1190.5	3118.5	164.8	1191.4	3078.4	133.1	1170.2	3079.0
161.7	1191.2	3105.9	142.8	1192.2	3120.8	182.9	1193.5	3081.8	147.9	1181.5	3081.5
177.2	1286.1	3106.5	160.0	1270.7	3131.2	189.7	1194.7	3099.9	164.8	1188.5	3098.4
193.1	1353.7	3129.5	172.6	1373.7	3138.2	234.6	1316.4	3107.5	181.2	1191.3	3101.1
206.2	1387.4	3138.3	190.9	1375.6	3140.7	265.7	1375.4	3109.6	188.1	1193.2	3109.5
234.6	1397.4	3140.4	211.7	1388.6	3165.6	277.1	1440.2	3111.1	190.3	1194.5	3110.6
263.0	1415.7	3154.4	247.3	1399.1	3266.5	313.1	1479.0	3124.1	234.9	1319.6	3115.5
391.3	1472.2	3229.6	320.9	1477.5	3310.9	343.2	1483.6	3163.9	264.4	1375.6	3125.3
425.2	1478.4	3354.2	330.5	1480.9	3434.0	364.2	1488.9	3389.3	274.2	1437.9	3164.5
478.4	1480.5	3461.9	457.5	1485.9	3699.2	465.5	1489.9	3857.7	313.2	1478.3	3397.2
512.8	1487.9	3843.0	490.5	1489.6	3875.2	469.5	1491.8	3884.9	339.7	1483.2	3857.1
									367.2	1488.8	3884.7
									382.2	1489.7	4335.2
CHTS2			CHp2			OHTS2			OHp2		
-949.9	483.1	1505.0	20.8	487.7	1503.1	-1220.6	518.8	1506.8	21.8	578.0	1492.9
61.6	604.2	1507.9	26.9	508.8	1503.9	51.3	573.7	1512.9	35.8	589.6	1496.3
74.4	720.8	1509.1	35.2	535.6	1506.4	60.4	770.7	1513.7	37.7	823.5	1504.2
83.2	883.4	1513.0	49.1	832.8	1513.3	70.7	879.4	1514.3	44.7	837.3	1506.2
93.6	933.2	1517.2	59.1	875.1	1515.9	82.7	925.8	1516.7	56.9	1019.1	1515.3
103.5	975.8	1518.3	63.5	1027.3	1517.6	88.0	970.4	1520.8	61.3	1034.9	1516.6
110.8	1016.2	1520.6	66.6	1063.2	1519.5	89.8	985.2	1523.8	67.1	1062.4	1517.9
119.5	1034.2	1528.4	75.1	1092.7	1524.8	107.8	1051.6	1526.8	71.6	1070.8	1518.5
129.1	1042.4	1532.8	78.8	1093.7	1547.4	115.3	1076.8	1532.8	75.5	1082.8	1525.9
142.7	1049.3	1537.2	85.8	1104.1	1566.5	119.1	1081.9	1537.2	85.5	1085.5	1528.7
148.0	1059.8	1550.6	89.6	1110.5	1610.9	145.9	1089.2	1548.4	88.5	1093.2	3037.7
157.6	1129.6	1625.7	96.8	1115.4	2536.3	151.7	1098.0	2921.8	94.4	1093.9	3038.6
177.4	1143.0	2828.9	99.1	1129.1	2798.3	164.3	1123.2	2944.2	97.3	1113.1	3041.4
178.7	1160.0	2863.6	102.5	1156.8	2932.5	168.3	1129.0	2946.1	98.7	1151.6	3050.2
195.8	1180.5	2936.9	110.5	1173.2	2940.5	179.8	1176.2	2952.7	116.3	1153.2	3068.7
210.6	1193.3	2943.4	118.3	1176.5	3019.1	198.5	1179.4	2967.6	120.8	1180.8	3098.0
224.2	1209.9	2944.9	135.4	1188.7	3025.5	203.6	1189.9	2990.5	130.1	1187.6	3099.0
240.1	1211.5	2951.7	139.6	1189.9	3031.5	251.7	1208.2	2998.2	140.0	1189.7	3103.5
260.7	1212.5	2993.1	145.0	1192.6	3047.6	261.4	1209.7	3005.0	177.9	1190.2	3112.0
283.6	1213.2	2994.7	150.0	1195.3	3065.1	267.1	1210.8	3008.6	183.1	1225.3	3126.2
316.7	1216.9	2999.3	168.1	1211.9	3074.4	291.5	1211.1	3026.6	192.0	1375.6	3128.1
318.0	1240.6	3012.2	183.4	1282.2	3089.3	293.8	1279.4	3030.4	231.2	1391.7	3134.5
334.0	1287.3	3012.4	207.5	1309.7	3095.7	295.2	1392.4	3037.3	261.3	1403.3	3150.2
337.6	1335.6	3018.5	219.9	1374.7	3101.8	297.8	1394.9	3038.9	271.2	1423.7	3164.8
338.4	1399.0	3026.8	245.4	1437.5	3109.1	301.5	1446.7	3061.0	302.9	1437.3	3233.2
346.1	1414.9	3042.6	256.2	1478.6	3118.2	347.6	1477.5	3076.9	420.6	1472.5	3254.9
370.0	1441.8	3109.7	290.9	1483.0	3165.9	415.6	1500.0	3234.7	466.9	1478.5	3403.2
390.2	1492.2	3277.5	304.6	1487.1	3405.7	447.8	1500.8	3317.7	472.6	1487.4	3438.5
437.6	1498.2	3643.1	371.7	1489.3	3849.9	479.1	1504.0	3724.4	496.2	1489.5	3487.2
470.9	1500.6	3727.9	462.7	1489.8	3891.3	488.3	1505.0	3809.4	503.7	1491.1	3882.3

Table S13. Harmonic vibrational frequencies (cm^{-1}) for the reactants, products, and intermediates of the $Li(NH_3)_4 + 2\ C_2H_4 \rightarrow Li(NH_3)_4 + C_5H_8O_2$ reaction pathway.

$Li(NH_3)_4$			CO_2r			eTS			CO_2p		
58.2	324.3	1646.1	15.4	329.1	1643.2	-796.2	323.4	1651.3	11.7	350.3	1665.6
64.5	407.3	1646.1	22.2	342.9	1647.2	19.7	329.6	1653.0	30.4	377.0	1666.0
64.8	407.4	1646.1	38.4	346.6	1647.6	39.7	345.8	1657.2	41.9	397.0	1691.7
65.0	503.6	3407.9	51.5	413.6	1653.5	51.3	351.8	1658.7	63.4	423.5	1701.7
74.4	503.8	3408.0	53.5	423.3	1655.0	58.8	383.7	1658.7	69.2	500.1	1705.1
74.5	504.2	3408.0	64.5	499.6	2428.3	69.0	418.5	2270.2	107.1	556.7	1723.5
76.2	1147.8	3425.9	75.4	502.0	3390.9	82.6	450.5	3407.5	113.8	564.1	3212.3
76.4	1147.8	3527.4	79.7	513.1	3404.3	84.7	513.0	3413.3	122.9	575.8	3270.2
76.5	1147.8	3527.4	85.9	638.3	3421.4	88.8	526.5	3421.9	141.3	645.4	3307.1
239.0	1159.1	3527.4	86.0	641.9	3430.1	92.3	565.1	3448.1	184.8	747.5	3501.7
315.2	1638.5	3530.4	88.6	1153.1	3505.1	116.4	1142.9	3507.2	225.0	1130.0	3539.1
315.3	1638.5	3530.4	95.1	1156.2	3513.5	117.7	1159.3	3519.8	228.8	1213.2	3543.1
315.6	1644.3	3534.8	105.9	1161.1	3514.8	127.4	1168.0	3522.7	237.0	1233.5	3544.5
324.1	1644.3	3534.8	127.1	1168.5	3529.1	136.6	1184.0	3544.0	249.8	1250.9	3601.1
324.2	1644.3	3534.9	237.6	1389.8	3530.7	157.0	1217.4	3546.4	255.8	1346.3	3605.2
			317.2	1636.4	3532.3	209.2	1643.3	3549.7	265.7	1649.3	3605.8
			320.8	1636.6	3553.3	238.7	1645.1	3564.7	316.8	1653.8	3612.9
			326.1	1643.1	3554.2	315.9	1649.4	3565.6	321.7	1665.4	3613.3
EtR			EtTS1			EtP			EtR2		
18.9	555.1	3210.3	-340.1	529.0	3212.8	8.6	577.8	3538.8	14.1	433.0	1637.9
25.6	565.1	3230.5	10.9	566.0	3246.3	16.5	586.5	3544.4	17.0	454.8	1649.0
32.6	583.8	3235.8	34.1	578.0	3319.1	22.4	595.5	3545.3	23.6	520.6	1660.3
39.3	646.7	3284.6	37.7	631.3	3326.7	40.7	644.2	3601.5	26.1	525.2	1665.2
47.2	748.2	3337.3	45.5	722.7	3368.8	44.2	675.3	3608.1	29.6	569.1	1665.7
53.8	855.2	3501.7	51.1	797.6	3501.4	54.3	879.6	3608.2	42.2	573.3	1670.1
58.8	998.9	3532.9	70.4	825.4	3539.5	69.5	931.5	3615.0	45.0	583.4	1697.2
71.3	1038.0	3539.6	71.2	919.8	3546.6	108.4	1015.0	3615.1	49.0	595.1	1712.7
74.5	1094.8	3545.2	112.8	1003.6	3547.6	111.7	1123.8	3132.0	55.6	643.4	1714.0
99.8	1129.9	3598.8	115.3	1131.2	3604.8	121.2	1124.1	3167.1	57.9	673.8	1721.1
108.5	1211.2	3602.0	120.3	1215.6	3605.6	166.8	1188.1	3185.2	71.6	855.1	3004.1
122.8	1229.7	3605.7	135.6	1221.0	3606.3	175.1	1217.3	3234.2	95.8	880.9	3013.4
124.1	1247.3	3612.5	165.9	1242.2	3612.4	199.8	1244.6	3277.9	110.8	932.1	3130.3
136.2	1262.3	3613.7	191.9	1250.1	3612.9	231.2	1267.2	3502.7	116.9	993.0	3148.8
169.7	1351.1		206.6	1289.4		246.6	1328.5		122.1	1015.4	3156.4
177.3	1394.8		213.9	1326.1		252.0	1434.6		167.4	1042.3	3168.0
219.1	1491.0		216.1	1467.9		279.7	1443.8		173.4	1100.2	3207.9
231.1	1652.9		224.0	1578.7		284.2	1456.9		179.3	1123.8	3222.9
240.5	1655.0		234.9	1642.1		317.0	1638.3		191.4	1124.2	3233.1
246.7	1665.7		249.4	1650.6		320.4	1649.2		227.2	1189.7	3267.2
265.2	1665.9		314.7	1660.7		322.2	1660.7		244.9	1216.3	3278.7
265.9	1666.8		319.0	1666.0		359.4	1665.1		251.4	1242.0	3502.6
318.3	1691.8		355.7	1666.2		383.2	1665.5		276.1	1261.3	3539.8
322.2	1700.9		380.0	1686.2		398.1	1670.8		284.1	1262.6	3542.1
355.1	1705.1		407.4	1696.3		433.1	1698.9		317.8	1328.4	3545.9
380.9	1710.5		414.4	1703.6		454.0	1714.5		318.7	1394.8	3602.3
408.5	1720.5		427.0	1770.7		519.5	1722.8		322.6	1435.4	3606.0
429.4	3132.0		476.4	3140.7		526.4	3004.4		361.4	1444.1	3609.4
500.7	3150.3		492.2	3158.0		565.4	3013.0		390.7	1455.8	3614.3
									401.1	1492.4	3615.3
EtTS2			EtP2			LacTS			LacP		
-461.7	518.2	1593.1	11.5	520.1	1670.1	-981.3	557.9	1494.9	11.2	513.2	1532.2
11.6	523.0	1634.1	15.6	539.9	1699.0	14.0	563.7	1506.0	20.3	530.8	1636.1
19.1	565.6	1649.7	22.4	566.6	1715.5	21.1	585.2	1645.5	35.4	572.7	1639.4
21.0	570.2	1660.0	34.6	578.9	1722.5	24.6	609.1	1654.9	39.8	587.9	1644.8
34.6	579.3	1665.4	36.4	588.7	1507.9	37.8	649.4	1664.5	51.4	719.6	1646.3
43.9	583.7	1665.7	47.6	601.5	1630.0	49.3	668.0	1665.4	71.2	773.7	1651.1

50.4	594.0	1670.9	65.0	662.5	1649.0	54.8	749.5	1666.6	74.0	821.5	1654.7
65.4	656.6	1698.2	73.5	710.4	1659.2	68.1	814.7	1701.4	79.4	889.2	1659.5
68.4	680.2	1715.1	91.1	738.0	1665.0	104.1	847.0	1711.3	84.7	953.0	1681.3
87.2	783.0	1721.3	107.2	851.1	1665.4	109.7	864.4	1723.9	96.2	975.2	1817.9
109.5	833.6	2993.5	108.7	905.2	2951.5	111.6	968.3	3015.2	102.4	992.8	3057.1
112.5	864.8	3063.6	115.4	941.3	3009.3	139.2	979.8	3027.6	110.3	1103.2	3065.1
120.1	881.0	3142.9	129.8	1050.7	3046.7	170.9	996.9	3039.3	136.5	1117.5	3068.9
162.5	911.7	3145.9	138.4	1078.7	3062.8	221.7	1035.9	3050.9	140.2	1127.8	3081.3
171.2	1001.3	3151.1	197.3	1100.2	3069.8	230.0	1089.7	3065.2	143.1	1129.6	3102.7
196.7	1032.7	3155.1	201.4	1123.4	3099.6	243.3	1104.1	3080.2	152.8	1138.8	3121.4
219.5	1036.8	3199.6	218.6	1135.6	3123.6	255.2	1119.7	3087.8	189.7	1147.8	3140.5
240.2	1123.5	3221.5	242.7	1163.9	3156.6	278.0	1211.8	3119.8	242.4	1158.1	3148.7
249.0	1125.9	3245.8	252.5	1217.2	3180.4	281.0	1223.6	3127.2	302.6	1186.6	3397.9
255.9	1213.6	3246.9	282.4	1245.1	3229.7	299.6	1233.2	3193.5	316.3	1233.2	3407.6
277.8	1216.8	3249.5	286.6	1265.9	3253.0	315.7	1237.2	3250.5	333.3	1280.6	3424.6
284.7	1242.4	3502.5	317.0	1269.3	3502.7	319.6	1249.3	3503.1	335.3	1300.2	3453.0
315.3	1252.1	3538.5	321.9	1289.4	3538.4	360.7	1262.0	3539.1	337.9	1303.7	3502.4
317.8	1265.8	3544.9	333.4	1326.8	3544.5	383.5	1289.1	3542.5	370.2	1357.6	3513.5
322.8	1307.4	3545.8	360.7	1354.9	3545.3	395.5	1343.1	3543.9	389.2	1393.6	3530.5
359.0	1333.5	3601.0	372.0	1411.0	3601.2	419.2	1369.5	3600.8	434.8	1398.7	3538.4
383.1	1437.6	3608.0	384.5	1453.1	3608.2	423.4	1385.3	3607.6	443.9	1431.7	3542.1
384.2	1456.1	3608.4	398.4	1470.9	3608.5	447.1	1467.3	3607.9	449.5	1486.5	3558.1
397.6	1461.7	3614.3	433.4	1473.3	3615.1	488.1	1479.2	3615.1	461.1	1495.4	3565.0
433.1	1482.0	3614.6	480.1	1475.9	3615.1	533.8	1489.4	3616.8	508.0	1521.4	3600.3
C_2H_4			δ-lactone								
842.0			96.4	1007.7	1474.5						
991.8			147.1	1082.2	1496.6						
1010.2			324.8	1132.0	1512.7						
1072.4			420.0	1138.1	1531.2						
1254.7			463.8	1192.9	1850.9						
1391.0			510.2	1218.3	3047.5						
1483.9			571.9	1282.8	3048.9						
1719.2			668.6	1296.1	3056.2						
3147.1			768.4	1317.8	3060.8						
3163.9			844.1	1377.4	3100.0						
3219.5			897.4	1390.8	3103.1						
3245.9			949.8	1404.6	3125.5						
			957.0	1443.5	3131.7						

Table S14. Harmonic vibrational frequencies (cm^{-1}) for the reactants, products, and intermediates of the $Li(NH_2CH_3)_4 + 2\ C_2H_4 \rightarrow Li(NH_2CH_3)_4 + C_5H_8O_2$ reaction pathway.

$Li(NH_2CH_3)_4$			CO_2r			eTS			CO_2p		
31.6	993.0	1651.7	14.6	554.9	1511.7	-382.4	507.8	1511.2	18.5	603.8	1513.1
32.0	997.9	3038.8	23.8	581.9	1522.2	19.8	536.7	1522.5	23.5	745.3	1523.6
33.4	1001.9	3039.1	25.6	958.1	1523.8	26.3	948.6	1524.9	41.1	934.7	1528.4
34.3	1058.2	3041.3	31.9	964.4	1526.6	31.6	971.4	1526.4	49.9	984.7	1529.5
45.3	1060.4	3041.9	33.8	969.3	1527.8	33.3	975.3	1528.5	51.8	987.2	1531.2
56.9	1062.5	3099.9	37.4	989.8	1617.5	39.0	989.2	1621.3	69.3	996.7	1663.5
65.3	1063.5	3100.1	40.4	993.5	1640.4	51.9	996.4	1641.2	77.3	999.1	1680.1
75.5	1207.5	3105.7	48.4	998.2	1650.3	54.0	997.9	1656.4	79.7	1045.3	1695.7
75.7	1207.7	3106.5	53.9	998.7	1662.7	55.6	1005.2	1667.7	86.7	1058.0	1697.5
97.1	1215.4	3123.7	65.1	1004.9	2423.6	59.8	1013.2	2353.3	101.8	1065.8	1711.6
129.2	1218.4	3124.1	68.8	1057.6	3038.1	65.4	1058.5	3040.4	103.5	1067.8	3032.8
135.0	1351.5	3132.5	73.4	1060.0	3040.5	70.9	1060.8	3040.8	110.6	1072.8	3034.6
135.1	1352.7	3133.0	82.9	1063.3	3041.2	81.4	1064.6	3041.2	133.3	1081.4	3035.9
166.0	1353.9	3381.4	97.2	1066.5	3042.5	95.8	1068.2	3042.5	138.2	1089.0	3040.1
168.7	1355.4	3389.4	111.0	1207.4	3099.1	98.5	1203.9	3099.8	140.5	1199.8	3083.7
181.6	1457.8	3430.2	114.6	1210.3	3102.5	125.4	1212.9	3100.3	155.2	1228.6	3086.5
208.4	1458.2	3448.2	133.2	1216.1	3103.4	130.5	1218.9	3102.0	164.9	1235.6	3087.7
233.6	1465.2	3450.8	147.8	1220.0	3107.0	137.5	1223.0	3108.1	170.5	1241.0	3108.5
355.5	1467.9	3456.6	160.9	1352.4	3121.8	146.2	1297.5	3123.1	177.4	1349.0	3122.3
374.7	1504.4	3536.2	179.4	1353.0	3129.9	166.8	1352.6	3130.1	197.7	1353.0	3128.0
402.5	1504.5	3536.4	187.5	1354.0	3130.9	173.7	1354.3	3132.9	215.3	1376.7	3135.7
437.4	1507.6		199.6	1358.7	3133.8	186.7	1356.4	3135.5	229.7	1380.9	3136.9
475.6	1509.4		239.9	1379.8	3375.5	210.5	1362.4	3337.8	238.0	1397.0	3284.9
491.3	1521.9		372.4	1457.7	3394.1	236.0	1458.1	3377.6	248.4	1467.2	3311.5
496.2	1522.1		392.6	1460.9	3430.2	366.6	1461.8	3449.6	374.0	1468.3	3343.4
956.9	1524.2		399.3	1466.0	3452.6	373.2	1467.4	3483.0	405.7	1469.0	3523.9
959.9	1526.5		441.0	1468.9	3460.6	394.7	1470.7	3488.4	456.8	1471.7	3551.4
964.3	1618.2		463.9	1504.1	3495.9	420.3	1504.0	3493.9	507.8	1508.6	3553.7
990.9	1638.3		497.4	1504.5	3540.4	442.4	1507.2	3561.1	521.0	1509.6	3554.7
991.2	1645.6		514.5	1507.8	3559.6	491.1	1508.5	3561.7	543.4	1512.0	3592.0
EtR			EtTS1			EtP			EtR2		
18.1	990.4	3040.4	-351.7	984.2	3034.2	12.8	988.0	2988.1	14.1	614.4	1507.0
24.6	998.9	3081.1	13.0	987.0	3035.0	16.4	999.1	3028.7	17.8	657.9	1508.7
27.1	1007.1	3086.6	18.9	998.0	3040.2	23.2	1001.7	3029.3	18.3	852.6	1512.1
30.5	1040.5	3091.3	31.8	1000.5	3041.1	35.9	1016.3	3030.8	22.3	876.8	1513.8
39.6	1043.2	3109.3	33.6	1010.5	3085.1	44.2	1056.7	3031.1	26.4	931.7	1523.1
43.8	1057.5	3117.7	40.3	1042.5	3087.9	48.0	1065.7	3038.5	36.1	933.2	1527.8
49.4	1065.6	3129.6	45.1	1057.3	3092.1	55.0	1067.4	3078.0	43.1	986.1	1530.1
53.9	1067.8	3134.5	56.1	1063.9	3110.9	64.5	1073.2	3079.6	45.1	987.9	1531.4
56.5	1072.6	3135.7	72.5	1066.6	3125.0	70.1	1079.0	3083.6	47.4	992.3	1640.3
70.7	1081.5	3137.7	76.7	1071.0	3130.2	87.7	1089.7	3108.1	49.7	1000.6	1663.4
74.9	1087.2	3150.9	81.9	1081.2	3136.6	97.8	1102.2	3117.8	55.7	1007.6	1688.6
79.2	1092.4	3210.5	87.6	1088.5	3139.5	101.2	1124.2	3121.8	67.0	1017.8	1709.2
86.4	1200.4	3236.1	95.7	1201.2	3146.0	105.3	1188.4	3135.7	71.7	1039.5	1711.9
91.8	1228.4	3298.9	99.1	1228.4	3157.1	109.7	1199.0	3137.1	86.3	1054.7	1713.8
100.9	1239.8	3317.2	111.3	1239.2	3219.0	133.3	1232.2	3167.3	88.6	1065.4	2976.8
104.9	1246.8	3352.2	123.0	1240.2	3246.0	137.5	1246.1	3204.9	97.9	1066.8	3027.9
112.6	1259.1	3523.9	135.7	1251.0	3292.0	142.4	1248.9	3239.1	102.1	1073.4	3029.7
131.1	1350.2	3547.3	138.6	1295.6	3308.6	162.4	1328.9	3277.6	105.8	1078.1	3030.7
135.1	1352.9	3551.4	155.0	1325.6	3371.2	163.7	1352.4	3286.3	111.4	1088.1	3038.9
142.8	1374.7	3553.9	158.1	1353.0	3524.0	171.9	1380.3	3525.2	133.5	1096.5	3042.5
149.8	1382.5	3592.0	169.5	1376.4	3551.2	176.6	1391.4	3551.9	137.4	1100.4	3077.5
156.7	1393.4	3029.9	172.2	1380.9	3552.0	200.6	1406.9	3552.0	144.7	1123.6	3081.8
162.1	1395.9	3034.8	184.9	1395.8	3552.9	205.4	1434.7	3553.2	160.1	1187.5	3085.2
170.1	1467.6	3036.1	196.7	1467.0	3591.8	220.0	1444.2	3593.6	162.4	1199.6	3109.0
175.8	1467.8		207.8	1468.7		232.7	1457.1		163.3	1231.9	3115.6
195.4	1470.9		229.7	1469.4		246.3	1466.2		174.2	1246.7	3124.8
215.2	1472.1		245.5	1471.4		316.1	1467.3		175.4	1258.2	3132.6
225.1	1490.8		249.0	1472.9		374.2	1468.7		198.8	1260.9	3134.0

236.5	1507.7		379.3	1508.3		416.1	1471.5		203.2	1330.1	3137.9
249.0	1509.1		406.4	1510.7		455.1	1507.0		219.8	1352.5	3150.6
378.6	1512.0		421.8	1511.4		458.4	1508.7		230.7	1379.5	3168.8
410.3	1513.6		439.5	1512.8		510.3	1512.5		247.4	1392.9	3209.0
451.4	1523.8		468.0	1525.1		525.7	1513.0		314.9	1394.3	3226.2
508.0	1527.9		501.9	1526.8		531.9	1523.1		377.0	1406.5	3235.1
519.8	1530.0		516.9	1529.0		560.8	1527.8		419.2	1436.2	3250.7
547.7	1530.9		557.1	1530.6		594.6	1529.6		454.8	1445.0	3278.2
602.9	1663.5		598.8	1581.4		610.1	1532.3		455.7	1459.1	3295.0
745.7	1681.6		713.4	1663.8		653.5	1643.3		510.3	1467.1	3524.8
851.2	1696.4		822.1	1678.4		877.0	1663.5		524.3	1467.7	3546.9
935.7	1699.5		825.3	1696.0		931.2	1688.5		528.2	1469.6	3552.3
984.7	1709.5		919.5	1696.6		932.1	1706.6		563.5	1471.7	3553.3
987.6	1716.1		936.4	1745.6		986.1	1711.4		592.2	1491.7	3593.3
	EtTS2			EtP2			LacTS			LacP	
-460.8	669.3	1506.8	11.1	753.6	1491.1	-984.9	847.0	1495.1	17.8	920.0	1495.9
9.5	783.3	1508.7	20.3	855.3	1506.9	19.0	864.0	1504.7	19.9	927.1	1505.2
18.4	833.4	1512.3	22.2	894.3	1508.8	22.9	930.6	1506.0	25.0	948.5	1507.5
21.8	865.2	1513.0	27.5	932.6	1512.4	24.0	968.1	1507.6	33.6	986.3	1508.0
25.9	879.4	1523.2	40.9	953.7	1513.0	33.5	980.1	1509.4	35.8	987.7	1509.5
39.0	910.5	1527.8	46.4	986.3	1523.2	38.3	986.5	1511.9	43.6	994.4	1512.7
45.4	933.5	1529.6	50.4	988.0	1527.7	40.7	988.9	1523.2	56.6	1001.5	1523.1
48.8	986.1	1532.1	61.0	999.4	1529.5	52.2	997.1	1524.8	64.5	1002.8	1526.5
58.4	987.6	1592.9	69.3	1001.9	1532.3	53.3	998.2	1527.4	65.4	1033.6	1527.5
65.1	998.9	1639.8	81.3	1009.2	1633.2	63.6	1004.8	1530.0	71.7	1046.5	1529.9
70.7	1000.0	1663.5	87.5	1056.8	1663.5	75.3	1035.1	1663.9	78.0	1063.3	1663.0
86.3	1002.4	1688.2	96.1	1066.0	1688.8	78.5	1055.3	1691.2	99.8	1067.3	1685.7
88.7	1032.3	1707.2	100.2	1067.5	1707.8	83.4	1065.4	1703.9	108.2	1074.9	1695.3
97.6	1036.3	1711.0	100.8	1071.0	1711.8	100.3	1068.5	1716.7	124.0	1078.6	1703.4
100.1	1055.9	2994.9	108.6	1073.5	2979.3	107.7	1078.0	3015.7	128.4	1082.8	2907.6
105.8	1065.3	3029.4	116.5	1079.1	3025.6	127.7	1082.1	3025.0	134.4	1100.1	2994.2
110.3	1067.0	3030.0	132.9	1090.2	3028.7	129.2	1084.4	3026.8	146.2	1111.4	3024.8
132.1	1073.0	3032.2	133.2	1102.3	3029.3	134.1	1089.8	3028.0	147.6	1120.0	3027.7
136.5	1078.4	3039.2	137.2	1105.6	3031.0	140.9	1099.7	3029.4	155.5	1132.1	3028.6
141.3	1089.0	3062.8	142.1	1128.8	3038.7	143.3	1104.3	3037.5	172.2	1198.0	3035.8
160.0	1101.0	3079.0	162.4	1190.0	3042.4	148.3	1198.2	3040.2	191.0	1198.2	3036.9
161.6	1123.6	3080.7	163.3	1199.2	3056.4	181.7	1212.0	3051.1	211.5	1229.5	3039.1
164.4	1199.5	3085.3	177.0	1232.3	3078.1	187.2	1234.4	3065.6	227.0	1232.7	3070.2
175.0	1215.2	3108.5	199.9	1244.1	3079.9	215.0	1235.6	3074.4	231.6	1239.0	3070.9
198.3	1231.5	3117.8	204.9	1246.8	3083.0	231.5	1239.2	3076.4	243.3	1246.2	3073.8
203.1	1245.5	3122.3	220.4	1249.8	3083.8	239.7	1248.4	3082.8	245.4	1282.0	3079.5
219.2	1248.6	3135.3	229.3	1315.3	3098.4	250.7	1258.0	3087.9	341.6	1311.5	3081.3
222.9	1252.1	3137.3	243.1	1337.6	3108.1	279.3	1289.3	3106.2	365.2	1343.7	3082.7
240.2	1307.4	3146.3	254.7	1352.5	3117.6	375.6	1342.5	3109.9	410.9	1352.9	3098.9
256.3	1333.6	3151.1	303.2	1352.7	3121.5	415.8	1351.8	3111.8	417.4	1376.2	3108.8
311.3	1352.6	3155.4	374.5	1380.4	3134.9	429.1	1369.7	3113.1	445.4	1380.4	3114.4
374.9	1379.7	3210.3	389.2	1392.0	3137.1	445.6	1381.4	3119.6	464.2	1385.5	3116.0
384.0	1391.1	3221.9	417.1	1407.5	3154.9	468.4	1385.3	3130.3	474.8	1393.0	3116.9
417.2	1406.2	3246.4	458.8	1411.4	3197.4	488.2	1385.8	3135.2	485.5	1398.8	3122.7
457.1	1437.0	3248.3	492.2	1454.8	3237.4	494.8	1397.5	3173.0	515.3	1418.3	3139.2
509.2	1455.7	3249.7	512.1	1466.3	3250.2	533.2	1464.5	3193.4	529.4	1465.3	3228.7
523.7	1461.4	3291.7	528.5	1467.2	3283.9	575.3	1467.6	3297.4	566.1	1467.5	3372.7
529.2	1466.6	3524.7	562.5	1468.5	3525.0	609.7	1468.8	3525.4	614.3	1467.7	3525.1
560.7	1467.5	3551.1	571.0	1470.4	3551.3	623.9	1471.6	3553.8	617.3	1471.1	3553.2
572.9	1469.0	3552.1	599.2	1471.4	3551.9	649.9	1473.4	3554.5	734.5	1471.2	3555.3
590.9	1471.8	3553.3	614.1	1471.8	3553.1	748.2	1479.4	3555.6	837.9	1487.0	3558.6
613.6	1481.8	3593.0	657.7	1475.8	3593.4	813.8	1489.7	3593.7	871.2	1487.5	3594.5
	OHTS			OHEtP							
-1820.4	608.4	1510.5	9.6	598.8	1512.9						
21.1	629.5	1513.1	16.5	629.3	1515.3						
24.1	657.9	1514.4	36.3	636.0	1525.9						
30.0	797.9	1523.7	44.4	846.4	1526.6						

42.0	1353.4	1529.2	51.6	881.4	1527.3						
46.6	1375.2	1530.2	55.8	939.4	1527.8						
51.4	877.8	1531.9	64.9	949.0	1532.3						
63.6	937.0	1629.2	68.4	964.7	1662.9						
74.2	983.2	1663.8	71.9	985.7	1673.7						
79.1	987.1	1679.3	81.8	1000.8	1687.0						
87.3	996.3	1696.6	88.5	1008.1	1699.4						
95.2	997.7	1700.2	98.3	1023.7	1701.1						
99.8	1041.4	1814.7	112.4	1026.2	3012.5						
112.1	1052.4	3034.6	116.1	1063.3	3028.3						
132.9	1054.9	3035.7	120.8	1068.7	3031.8						
138.4	1063.5	3038.1	130.4	1071.2	3032.6						
144.0	1066.1	3041.3	140.9	1078.8	3078.5						
159.2	1071.0	3086.3	144.1	1085.8	3091.0						
164.3	1079.4	3089.1	162.7	1195.4	3094.7						
177.3	1086.2	3089.9	173.8	1200.0	3099.3						
193.4	1113.1	3109.3	186.0	1202.9	3110.2						
194.9	1200.6	3112.6	198.9	1208.4	3124.8						
210.4	1204.6	3123.9	210.1	1228.3	3133.9						
212.7	1227.7	3133.4	212.9	1243.9	3135.6						
226.2	1229.8	3137.6	236.8	1305.0	3145.3						
240.0	1239.1	3137.9	314.6	1363.5	3185.2						
278.1	1259.1	3164.6	339.1	1371.4	3243.5						
373.1	1377.1	3251.1	404.9	1373.8	3317.6						
373.7	1382.6	3338.5	417.4	1390.8	3403.3						
400.7	1396.0	3349.9	453.6	1401.8	3487.0						
457.8	1467.4	3378.8	467.1	1466.5	3493.0						
504.1	1468.8	3523.4	477.1	1467.4	3558.6						
518.0	1469.8	3552.2	492.8	1468.0	3578.5						
520.2	1472.0	3555.7	550.6	1469.6	3584.3						
535.8	1492.0	3556.7	575.9	1506.6	3585.9						
591.0	1509.2	3591.1	582.0	1507.8	3828.5						

Table S15. Electronic energy (a.u.) of the structures along the reaction pathway of Li(X) + CO_2 + $2H_2$→ $CH_2(OH)_2$ (X= NH_3, H_2O) at CCSD(T) with double-ζ basis sets, CC(DZ), and MP2 with double-ζ, MP2(DZ), and triple-ζ, MP2(TZ) basis sets. Values used in Figure S2 comparison of CCSD(T) and CAM-B3LYP energetics. R (reactants) denotes the energy of Li(X)••••CO2••••$2H_2$ and P (products) denotes the energy of Li(X)••••$CH_2(OH)_2$.

	$Li(NH_3)_4$			$Li(H_2O)_4$		
	CC(DZ)	MP2(DZ)	MP2(TZ)	CC(DZ)	MP2(DZ)	MP2(TZ)
R	-423.274095	-423.551664	-423.990146	-503.029912	-502.945839	-503.451355
CO_2r	-423.281832	-423.560060	-423.994565	-503.041491	-502.957009	-503.460124
eTS1	-423.276135	-423.554980	-423.988323	-503.034916	-502.950993	-503.453712
CO_2p	-423.297202	-423.571260	-424.011232	-503.061219	-502.974195	-503.482113
H_2r1	-423.301954	-423.576352	-424.014272	-503.065544	-502.978364	-503.484730
CHTS1	-423.276075	-423.552475	-423.989270	-503.041380	-502.954705	-503.459358
CHp1	-423.282672	-423.562866	-423.999220	-503.050582	-502.969871	-503.475534
OHTS1	-423.271586	-423.548744	-423.983504	-503.043849	-502.957320	-503.460456
OHp1	-423.289411	-423.562307	-423.997236	-503.053005	-502.964811	-503.468276
eTS2	-423.284432	-423.558764	-423.992419	-503.038758	-502.948669	-503.458690
rFA	-423.290013	-423.565533	-424.003691	-503.066456	-502.978298	-503.484929
H_2r2	-423.295253	-423.571044	-424.007143	-503.071763	-502.982890	-503.487640
CHTS2	-423.271939	-423.550625	-423.980691	-503.052037	-502.963847	-503.464475
CHp2	-423.269162	-423.551548	-423.984940	-503.055984	-502.972028	-503.473450
OHTS2	-423.271739	-423.550205	-423.983761	-503.050616	-502.963673	-503.465706
OHp2	-423.270014	-423.585334	-424.018990	-503.081938	-502.992714	-503.494038
P	-423.299005	-423.571885	-424.010266	-503.055130	-502.966060	-503.471475

Table S16. Electronic Energy, enthalpy, and free energy of the structures along the reaction pathway of Li(X) + CO_2 + $2H_2$→ $CH_2(OH)_2$ (X= NH_3, NH_2CH_3, $NH_2CH_2CH_3$, H_2O, CH_3OH) at CAM-B3LYP. These values were used for Figures 1 and 2.

	NH_3			NH_2CH_3			$NH_2CH_2CH_3$		
	-E(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)	-ΔE(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)	-E(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)
SEP	233.791296	233.628588	233.685142	390.937396	390.652391	390.722689	548.158864	547.754406	547.837160
CO_2r	422.388125	422.208546	422.278698	579.535766	579.233986	579.318450	736.757649	736.336501	736.433702
eTS1	422.384014	422.206543	422.273705	579.535152	579.235071	579.317255	736.758236	736.352103	736.446166
CO_2p	422.412669	422.232517	422.295955	579.569194	579.267218	579.344617	736.794357	736.373085	736.464362
H_2r1	423.586664	423.391189	423.461990	580.743026	580.425777	580.511292	737.966423	737.530224	737.629958
CHTS1	423.563052	423.371473	423.436791	580.719228	580.405773	580.484353	737.944393	737.511647	737.604986
CHp1	423.565437	423.369843	423.438101	580.719936	580.403035	580.486251	737.944722	737.508402	737.605719
OHTS1	423.554691	423.358742	423.423797	580.710363	580.392696	580.472594	737.935222	737.498234	737.592361
OHp1	423.567678	423.364832	423.433200	580.720160	580.395575	580.475892	737.943716	737.499924	737.594332
eTS2	423.564494	423.363855	423.429091	580.716958	580.394240	580.472818	737.938951	737.497282	737.589419
rFA	423.576776	423.374602	423.438293	580.732841	580.409023	580.488231	737.956990	737.513955	737.594332
H_2r2	424.751106	424.533524	424.604195	581.907087	581.567862	581.654103	739.130667	738.672172	738.771451
CHTS2	424.722451	424.508231	424.564835	581.877225	581.543121	581.611060	739.099626	738.647014	738.724337
CHp2	424.725178	424.506203	424.573212	581.882826	581.541545	581.623121	739.107030	738.646482	738.739469
OHTS2	424.724865	424.506481	424.572782	581.882679	581.542241	581.622982	739.105104	738.645801	738.741657
OHp2	424.760810	424.533473	424.603061	581.913563	581.563799	581.646154	739.136588	738.667409	738.762115
	H_2O			CH_3OH					
	-E(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)	-E(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)	-E(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)
SEP	313.309898	313.200937	313.253401	470.441637	470.210209	470.279448	H_2		
CO_2r	501.911645	501.785504	501.850687	659.041785	658.794569	658.875953	1.171609	1.158264	1.173063
eTS1	501.905457	501.781466	501.846342	659.039911	658.794824	658.864216	CO_2		
CO2p	501.942292	501.815733	501.873967	659.088960	658.839430	658.916336	188.594168	188.578722	188.603603
H_2r1	503.115884	502.974057	503.041186	660.262256	659.997551	660.083074	CH_2O_2		
CHTS1	503.093917	502.956540	503.016570	660.239641	659.979234	660.058200	189.766492	189.728539	189.756783
CHp1	503.098337	502.957102	503.021999	660.243997	659.979251	660.061155	$CH_2(OH)_2$		
OHTS1	503.089000	502.946247	503.004608	660.227007	659.961860	660.040089	190.963222	-190.900830	190.929872
OHp1	503.096933	502.947877	503.012022	660.232244	659.961255	660.041439	C_2H_4		
eTS2	503.092772	502.947725	503.000193	660.227057	659.957217	660.037009	78.567649	78.512323	78.537148
rFA	503.115568	502.966221	503.023576	660.259945	659.988375	660.065304	δ-Lactone		
H_2r2	504.289382	504.124420	504.191654	661.433604	661.146687	661.230956	345.774684	345.638959	345.676394
CHTS2	504.266175	504.105467	504.162149	661.402996	661.121391	661.188450			
CHp2	504.266844	504.100147	504.160364	661.407769	661.121121	661.203854			
OHTS2	504.263558	504.097058	504.154609	661.404633	661.117361	661.186232			
OHp2	504.292060	504.117668	504.178928	661.427702	661.131209	661.211058			

Table S17. Electronic energy, enthalpy, and free energy of the structures along the reaction pathway of Li(X) + 2 C_2H_4 + CO_2 → Li(X) + $C_5H_8O_2$ (X= NH_3, NH_2CH_3) at CAM-B3LYP. These values were used for Figure 3.

	NH_3			NH_2CH_3		
	-E(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)	-E(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)
SEP	233.791296	233.628588	233.685142	390.937396	390.652391	390.722689
CO_2r	422.388125	422.208546	422.278698	579.535766	579.233986	579.318450
eTS1	422.384014	422.206543	422.273705	579.535152	579.235071	579.317255
CO_2p	422.412669	422.232517	422.295955	579.569194	579.267218	579.344617
EtR	500.985266	500.747584	500.824017	658.140925	657.781531	657.873140
EtTS1	500.970722	500.734663	500.806279	658.126538	657.768802	657.855275
EtP	501.009877	500.772878	500.845225	658.165890	657.807098	657.893122
EtR2	579.581849	579.287298	579.373134	736.737279	736.320998	736.421424
EtTS2	579.567070	579.273026	579.351628	736.722832	736.307032	736.400141
EtP2	579.615371	579.318386	579.397846	736.771558	736.352643	736.444956
LacTS	579.555094	579.258380	579.331824	736.711077	736.292722	736.381259
LacP	579.575164	579.273583	579.350646	736.742512	736.320919	736.408466

Table S18. Electronic energy, enthalpy, and free energy of the structures along the reaction 1-4 (a.u.) and enthalpy/free energy of reaction (kcal/mol) at CAM-B3LYP. These values were used for Figure 4.

Reaction 1	-ΔE(a.u.)	ZPE(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)
CO_2	188.594168	0.011897	188.578722	188.603603
Ethene	78.567649	0.051353	78.512323	78.537148
δ-lactone	345.774684	0.128588	345.638959	345.676394
		Δ_{rxn}(kcal/mol)	-22.33	0.94
Reaction 2	-ΔE(a.u.)	ZPE(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)
CO_2	188.594168	0.011897	188.578722	188.603603
Butadiene	155.947359	0.085755	155.856017	155.887558
Product 2	344.545714	0.104155	344.434504	344.472513
		Δ_{rxn}(kcal/mol)	0.15	11.70
Reaction 3	-ΔE(a.u.)	ZPE(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)
CO_2	188.594168	0.011897	188.578722	188.603603
Octadiene	313.154281	0.200613	312.943015	312.989641
Product 3	501.789621	0.223032	501.556279	501.601205
		Δ_{rxn}(kcal/mol)	-21.68	-5.00
Reaction 4	-ΔE(a.u.)	ZPE(a.u.)	-ΔH(a.u.)	-ΔG(a.u.)
CO_2	188.594168	0.011897	188.578722	188.603603
O-Xylxylene	309.526744	0.133579	309.385561	309.423243
Product 4	498.167359	0.152600	498.005714	498.048092
		Δ_{rxn}(kcal/mol)	-26.00	-13.33

Table S19. Harmonic vibrational frequencies (cm^{-1}) for the reactants and products listed in Figure 4.

Product 4			C_2H_4			Butadiene			Octadiene		
75.9	892.9	1366.1	842.0	1254.7	3147.1	169.5	1035.3	1716.6	22.7	979.7	1487.9
149.8	926.3	1427.8	991.8	1391.0	3163.9	280.2	1050.9	1727.8	82.8	1020.4	1497.2
193.7	963.1	1470.0	1010.2	1483.9	3219.5	474.8	1082.2	3149.8	97.4	1045.2	1500.5
260.6	1005.0	1514.7	1072.4	1719.2	3245.9	634.0	1118.7	3156.4	100.0	1056.6	1502.5
340.3	1031.3	1520.2				771.3	1325.4	3160.4	164.0	1058.6	1737.4
399.7	1037.9	1553.2				896.2	1354.9	3168.9	256.9	1106.9	1739.2
436.6	1073.9	1670.0				976.8	1449.9	3242.4	282.9	1138.4	3026.2
471.3	1103.0	1692.2				978.9	1477.1	3243.9	358.3	1159.3	3030.7
515.7	1147.8	1864.6	CO_2						405.7	1238.5	3039.7
563.8	1180.1	3028.3	686.2	1399.5	2450.6				447.1	1247.8	3047.2
571.8	1190.4	3035.2	686.2						468.5	1290.4	3064.4
652.9	1222.5	3140.4							637.7	1309.4	3070.1
719.3	1253.6	3150.6							648.7	1336.4	3082.6
768.4	1264.4	3185.3							799.1	1338.2	3110.3
779.0	1284.1	3190.3							827.4	1370.1	3134.4
797.9	1302.9	3203.1							858.4	1379.7	3139.4
844.6	1334.5	3216.8							920.9	1400.9	3150.9
									948.6	1411.4	3151.3
									966.8	1466.0	3230.5
									971.0	1467.1	3230.8
O-Xylxylene			δ-lactone			Product 2			Product 3		
81.0	883.4	1462.9	96.4	1007.7	1474.5	42.5	978.0	1450.2	70.0	999.3	1425.3
232.7	946.1	1490.0	147.1	1082.2	1496.6	102.1	993.7	1465.7	112.6	1063.4	1447.9
353.9	949.5	1643.6	324.8	1132.0	1512.7	383.2	1023.8	1517.2	176.6	1080.6	1474.3
415.4	968.2	1672.4	420.0	1138.1	1531.2	457.2	1050.0	1783.9	197.1	1101.1	1498.6
438.1	981.2	1683.9	463.8	1192.9	1850.9	527.4	1150.9	1853.9	268.9	1107.4	1500.1
442.3	1020.5	1745.9	510.2	1218.3	3047.5	560.8	1184.8	3052.7	326.9	1140.1	1503.0
522.6	1023.1	3167.6	571.9	1282.8	3048.9	567.7	1238.2	3066.6	334.0	1148.4	1514.3
594.7	1027.3	3170.9	668.6	1296.1	3056.2	695.6	1274.9	3077.2	383.6	1165.6	1527.4
665.5	1196.5	3183.6	768.4	1317.8	3060.8	772.0	1283.0	3088.5	403.7	1179.8	1849.0
712.6	1197.7	3189.2	844.1	1377.4	3100.0	920.8	1380.1	3180.9	469.5	1216.8	3000.5
736.0	1275.1	3203.2	897.4	1390.8	3103.1	955.6	1437.7	3202.1	481.5	1243.0	3013.9
767.7	1346.2	3213.4	949.8	1404.6	3125.5				513.6	1266.8	3027.6
818.8	1391.3	3250.7	957.0	1443.5	3131.7				571.1	1269.2	3028.9
856.0	1458.5	3255.0							620.5	1299.3	3033.7
									718.2	1320.9	3040.0
									777.4	1321.2	3046.3
									816.5	1339.2	3051.3
									848.8	1364.9	3075.8
									877.1	1375.2	3076.5
									884.5	1390.9	3086.1
									947.2	1395.7	3088.5
									963.8	1405.3	3116.2
									980.5	1414.9	3122.4

Table S20. Cartesian Coordinates (Å) for the reactants and products listed in Figure 4.

CO_2				C_2H_4				Butadiene			
C	0.000000	0.000000	-0.000010	C	-0.000000	-0.000000	0.659538	C	-0.108097	-1.529297	-0.485144
O	0.000000	0.000000	-1.155618	C	0.000000	-0.000000	-0.659538	C	0.108097	-0.724870	0.545349
O	-0.000000	-0.000000	1.155626	H	0.000000	0.920763	1.227183	C	-0.108097	0.724870	0.545349
				H	-0.000000	-0.920763	1.227183	C	0.108097	1.529297	-0.485144
				H	0.000000	0.920763	-1.227183	H	-0.452814	1.153503	1.480108
				H	-0.000000	-0.920763	-1.227183	H	0.502934	1.155872	-1.420583
								H	-0.088835	2.589704	-0.420755
								H	0.088835	-2.589704	-0.420755
								H	-0.502934	-1.155872	-1.420583
								H	0.452814	-1.153503	1.480108
Octadiene				O-Xylxylene				δ-lactone			
C	-2.278629	0.218657	0.006590	C	-0.197770	1.475966	-1.717885	C	-1.719179	-0.061151	0.324971
C	1.737631	0.775799	-0.353278	C	0.008481	0.743026	-0.619850	C	-0.960800	-1.266976	-0.174499
C	-1.203205	-0.138792	0.982638	C	-0.008481	-0.743026	-0.619850	C	-1.117156	1.190316	-0.287626
C	1.743687	-0.705060	-0.566406	C	0.197770	-1.475966	-1.717885	H	-1.663922	-0.012132	1.414570
C	-0.451926	-1.421903	0.609473	C	0.197770	1.394957	0.671330	H	-2.769711	-0.175425	0.057485
C	0.365749	-1.365242	-0.681131	C	-0.197770	-1.394957	0.671330	C	0.349863	1.276046	0.106030
C	2.414032	1.416672	0.584136	C	0.123990	0.714433	1.818360	H	-1.643945	2.086779	0.036164
C	-2.394100	1.377485	-0.618531	C	-0.123990	-0.714433	1.818360	H	-1.212701	1.143328	-1.374682
H	-3.017281	-0.554698	-0.186648	H	-0.348294	-2.465998	0.671843	H	0.436216	1.582227	1.151411
H	-1.681950	2.177512	-0.458993	H	-0.229693	-1.226491	2.764453	H	0.899447	2.014301	-0.472297
H	-3.205698	1.573322	-1.305340	H	0.348294	2.465998	0.671843	C	1.129571	-0.017063	0.013435
H	-1.662918	-0.294025	1.962815	H	0.229693	1.226491	2.764453	O	0.455987	-1.183926	0.035733
H	-0.511181	0.694447	1.090727	H	-0.437332	1.030406	-2.671587	O	2.325566	-0.039155	-0.009721
H	0.204365	-1.700667	1.437116	H	-0.150350	2.554902	-1.676438	H	-1.125559	-1.402069	-1.245790
H	-1.184243	-2.228200	0.522356	H	0.437332	-1.030406	-2.671587	H	-1.266043	-2.179396	0.331168
H	2.317292	-1.184597	0.229988	H	0.150350	-2.554902	-1.676438				
H	2.282307	-0.905390	-1.497401								
H	0.523489	-2.386576	-1.031100								
H	-0.212984	-0.865693	-1.461358								
H	1.138909	1.349960	-1.054385								
H	3.022610	0.884666	1.304844								
H	2.387844	2.494244	0.666440								
Product 2				Product 3				Product 4			
C	1.069639	-1.233903	0.000100	C	0.802781	1.608974	0.205187	C	0.706685	1.591693	0.386642
C	1.770311	0.075465	0.000003	C	-0.342064	0.750756	-0.280099	C	-0.506266	0.743899	0.168037
C	1.130514	1.226854	-0.000073	C	-0.192834	-0.645061	0.312721	C	-0.325446	-0.628487	0.258764
C	-0.357996	1.294078	0.000046	C	1.150501	-1.216186	-0.111294	C	1.064252	-1.104129	0.564485
C	-1.074232	-0.034675	0.000021	C	2.331450	-0.276157	-0.028324	C	2.119841	-0.280054	-0.137460
H	-0.730601	1.844202	-0.865831	H	1.101930	-1.520717	-1.160716	H	1.223810	-2.143150	0.294635
H	-0.730440	1.844155	0.866029	H	1.418838	-2.108635	0.449906	H	1.259547	-1.017158	1.639117
H	2.851376	0.030984	0.000004	O	3.461961	-0.668530	-0.027249	O	3.127065	-0.735903	-0.590489
H	1.676160	2.161022	-0.000144	O	2.101002	1.051161	-0.033254	O	1.874103	1.040503	-0.237574
O	-2.268046	-0.105182	0.000030	H	0.709517	1.783178	1.280190	H	0.913941	1.712595	1.453822
O	-0.356770	-1.171052	-0.000164	H	0.816150	2.576830	-0.291290	H	0.591287	2.580367	-0.047106
H	1.351183	-1.818586	0.877917	C	-1.687478	1.374589	0.075516	C	-1.757004	1.266391	-0.109672
H	1.351439	-1.818819	-0.877476	H	-0.273904	0.666808	-1.370795	C	-1.400853	-1.477357	0.062559
				C	-1.355980	-1.548059	-0.080259	C	-2.835739	0.415925	-0.286891
				H	-0.200592	-0.538644	1.404068	C	-2.655957	-0.954623	-0.203235
				C	-2.846245	0.467364	-0.325000	H	-1.258152	-2.548324	0.115785
				H	-1.786038	2.350905	-0.402290	H	-3.494172	-1.619835	-0.354328
				H	-1.724498	1.549929	1.155029	H	-1.889340	2.337040	-0.193254
				C	-2.699211	-0.924540	0.281698	H	-3.813341	0.822121	-0.503540
				H	-1.245842	-2.524174	0.395375				
				H	-1.316602	-1.722691	-1.160049				
				H	-2.878431	0.383819	-1.414777				
				H	-3.792450	0.915053	-0.020205				
				H	-2.783793	-0.854130	1.369732				
				H	-3.513497	-1.568650	-0.051032				