

Azaaldol Condensation of a Lithium Enolate  
Solvated by *N,N,N',N'*-Tetramethylethylenediamine:  
Dimer-Based 1,2-Addition to Imines

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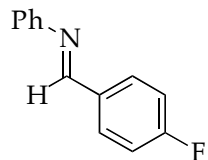
### Part 3: Computations

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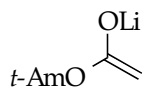
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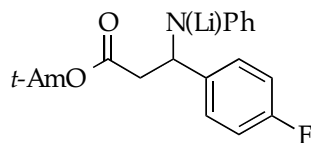
## Structure Numbers



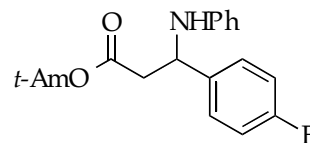
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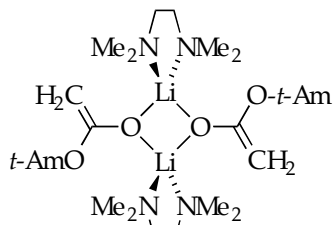
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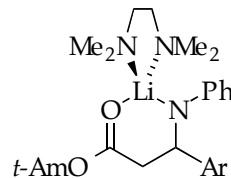
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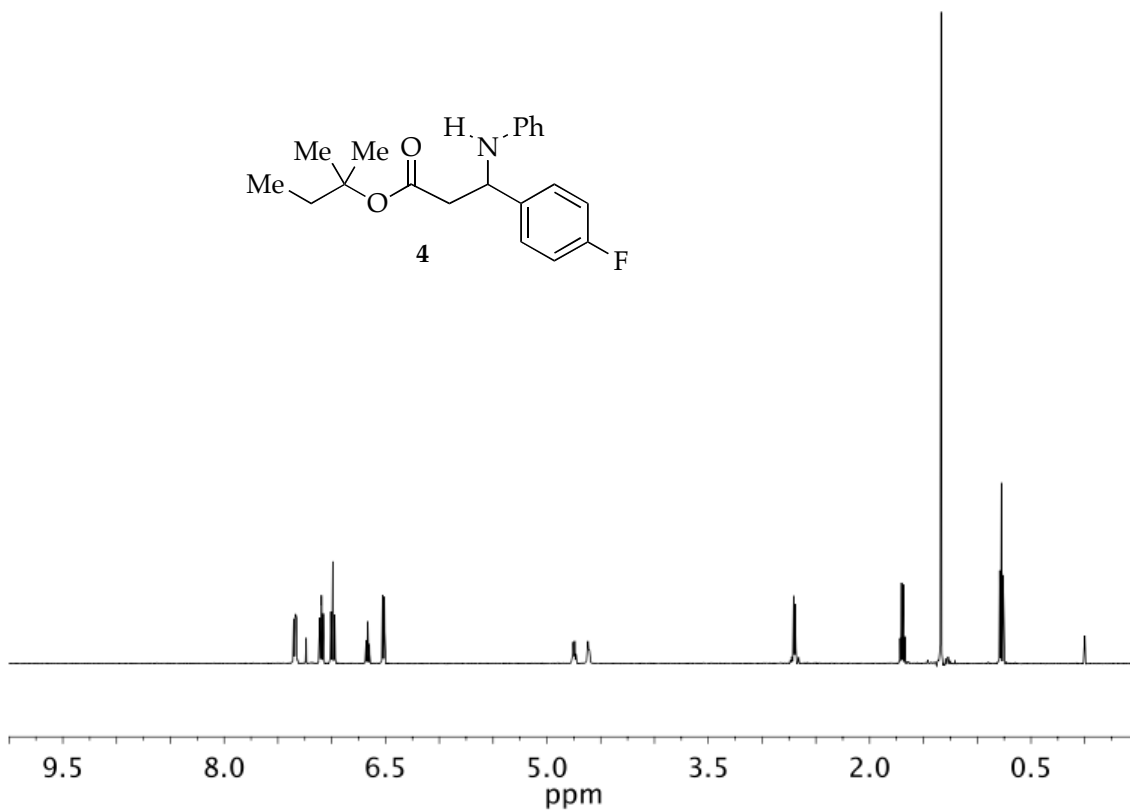
4



2a



3a



**Figure 1.** <sup>1</sup>H NMR spectrum of 4 in CDCl<sub>3</sub>.

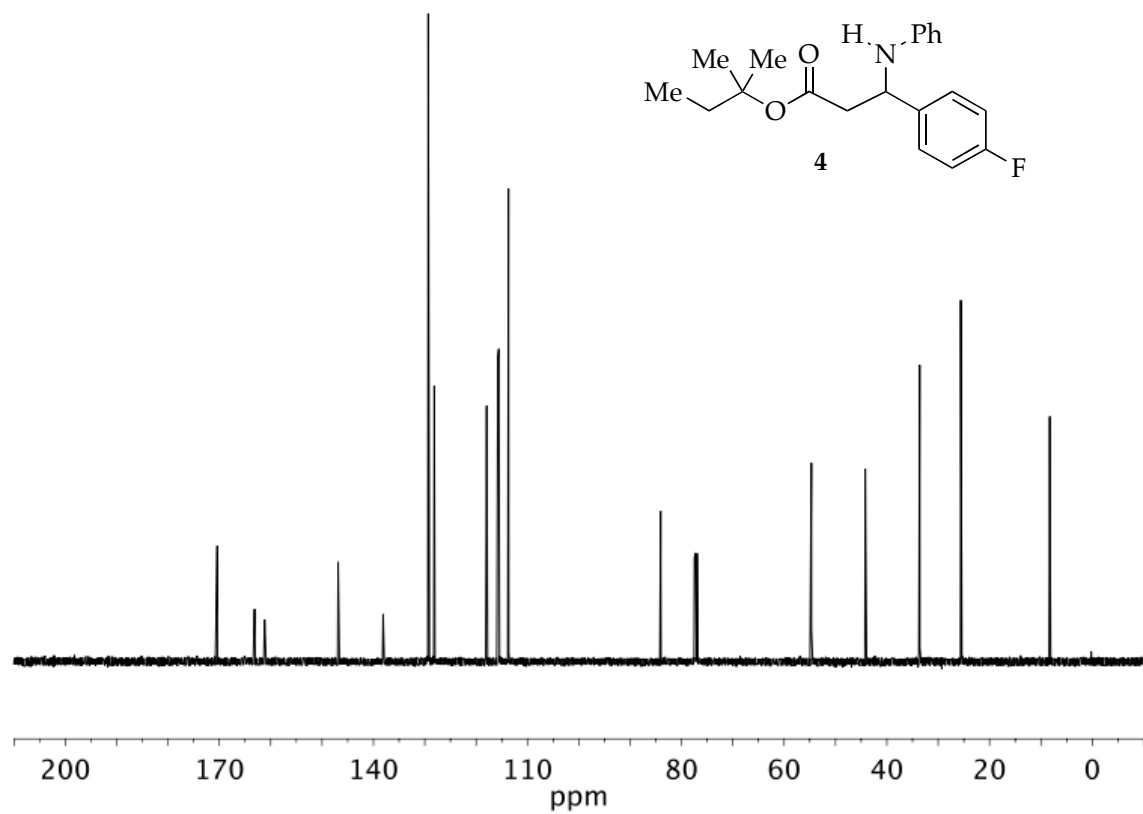
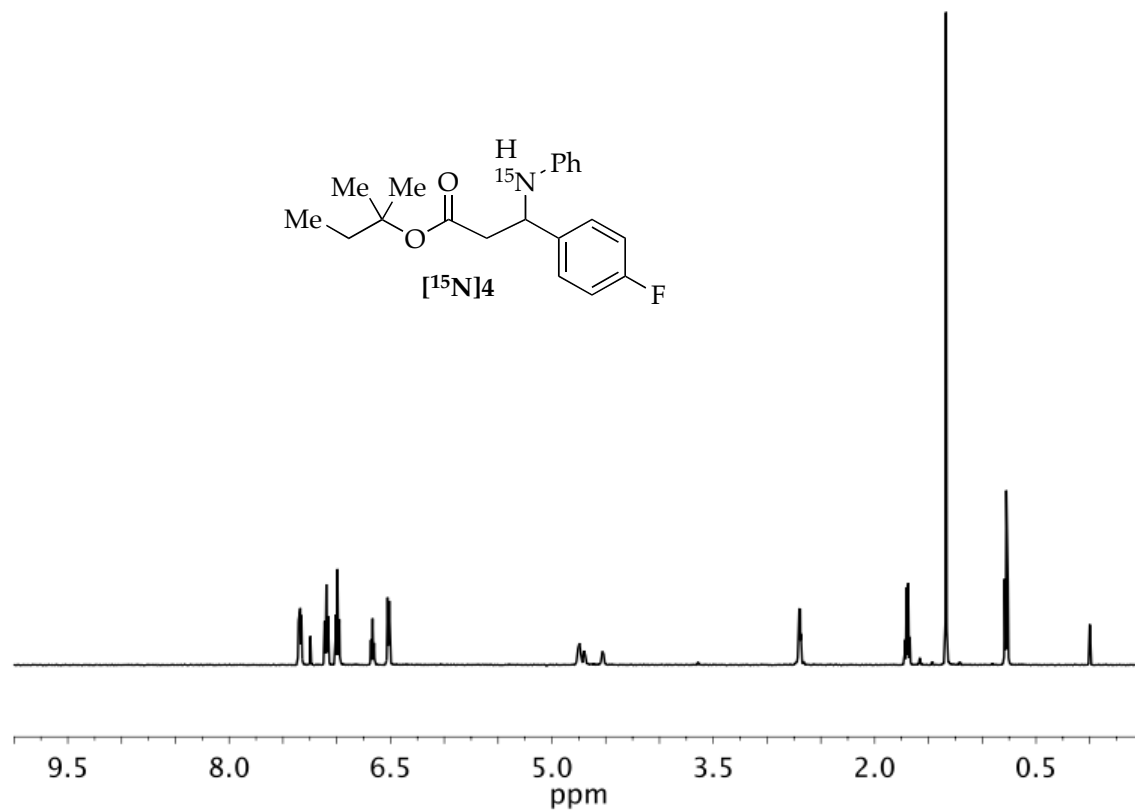
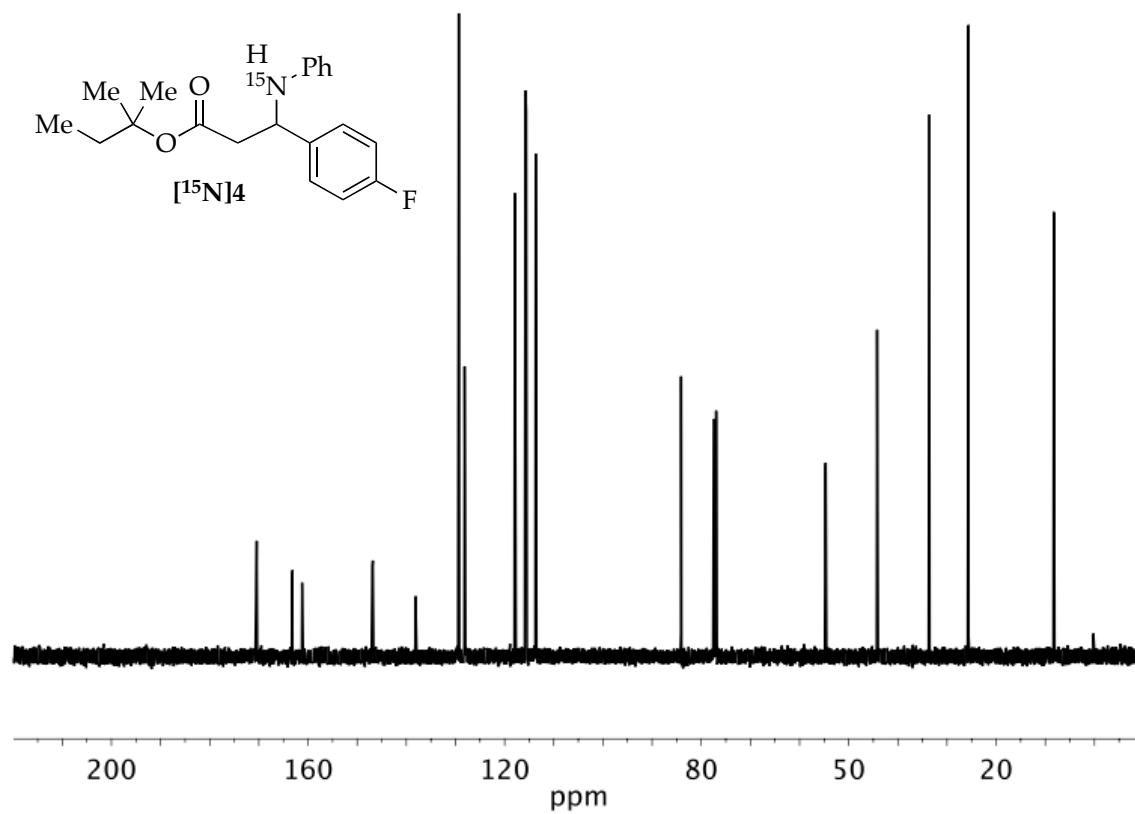


Figure 2. <sup>13</sup>C NMR spectrum of 4 in CDCl<sub>3</sub>.



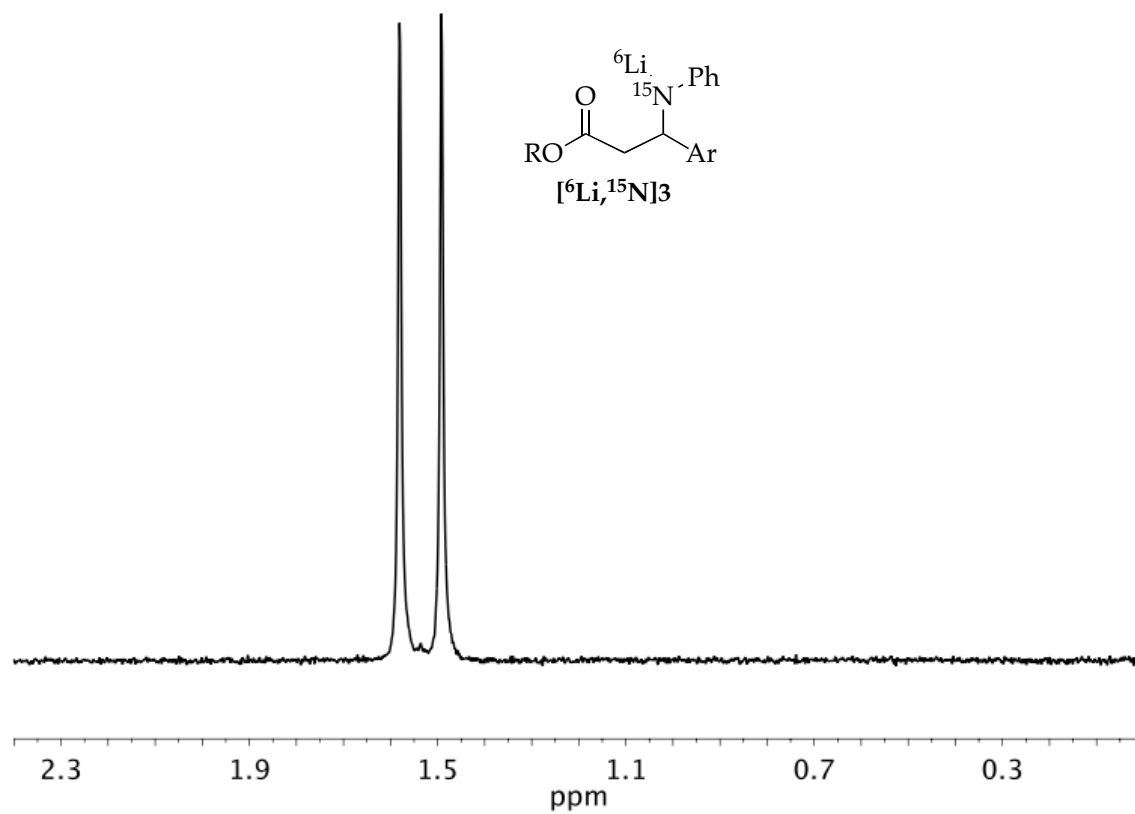
**Figure 3.**  $^1\text{H}$  NMR spectrum of  $[^{15}\text{N}]4$  in  $\text{CDCl}_3$ .

TDVa-300r-C-500  
TDVa-300r-C



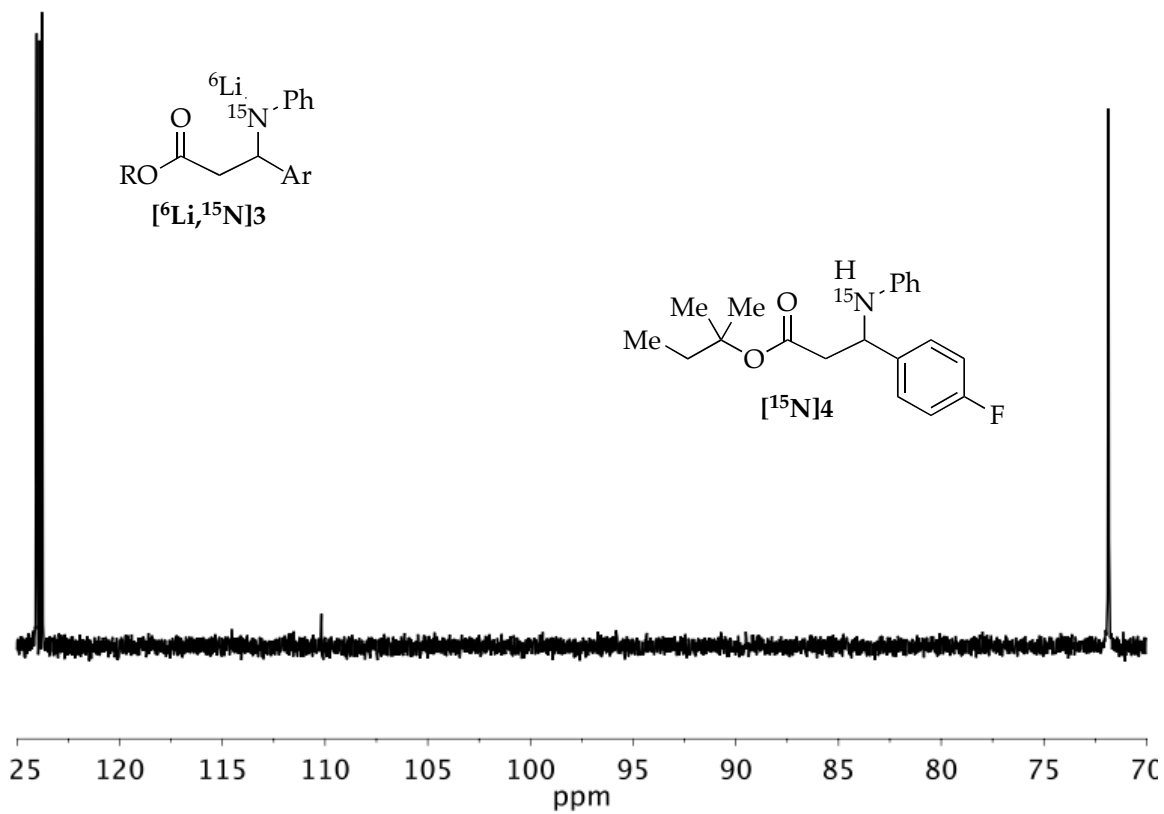
**Figure 4.**  $^{13}\text{C}$  NMR spectrum of  $[^{15}\text{N}]4$  in CDCl<sub>3</sub>.

TDVa-009q  
TDVa-009q

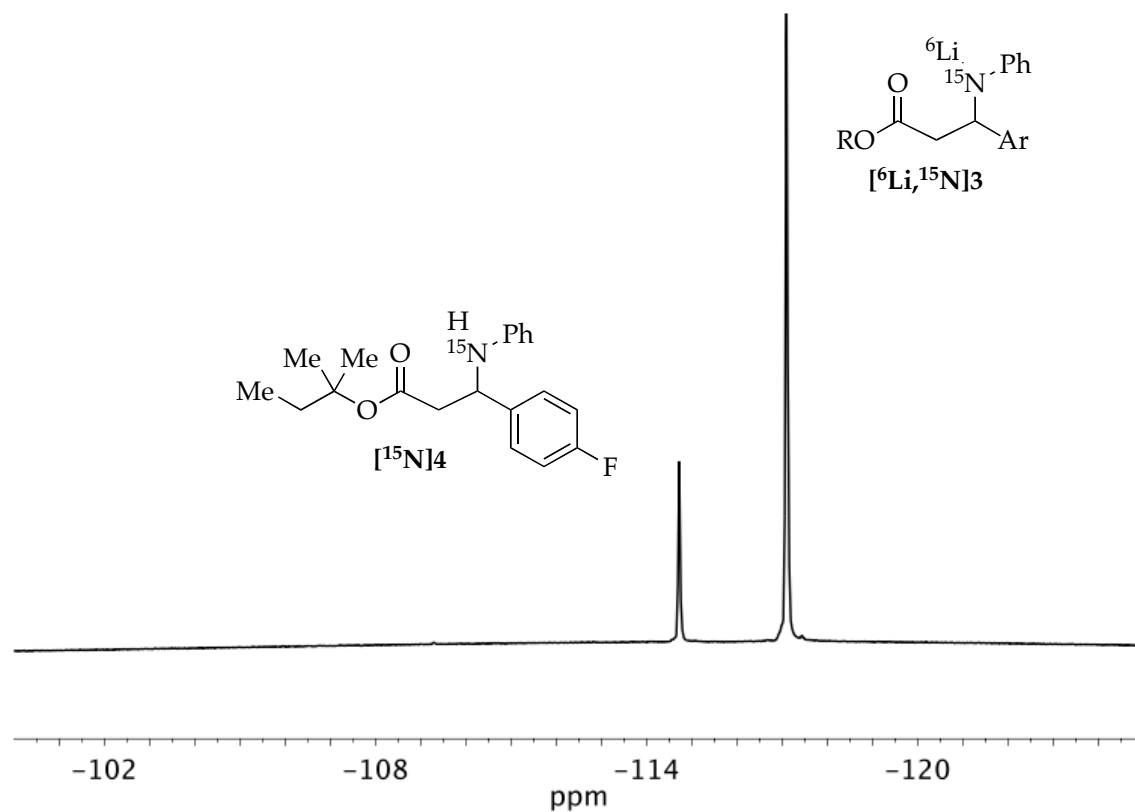


**Figure 5.**  $^6\text{Li}$  NMR spectrum of a 0.10 M solution of  $[^6\text{Li}, ^{15}\text{N}]_3$  in 0.60 M TMEDA/toluene at  $-60\text{ }^\circ\text{C}$ .

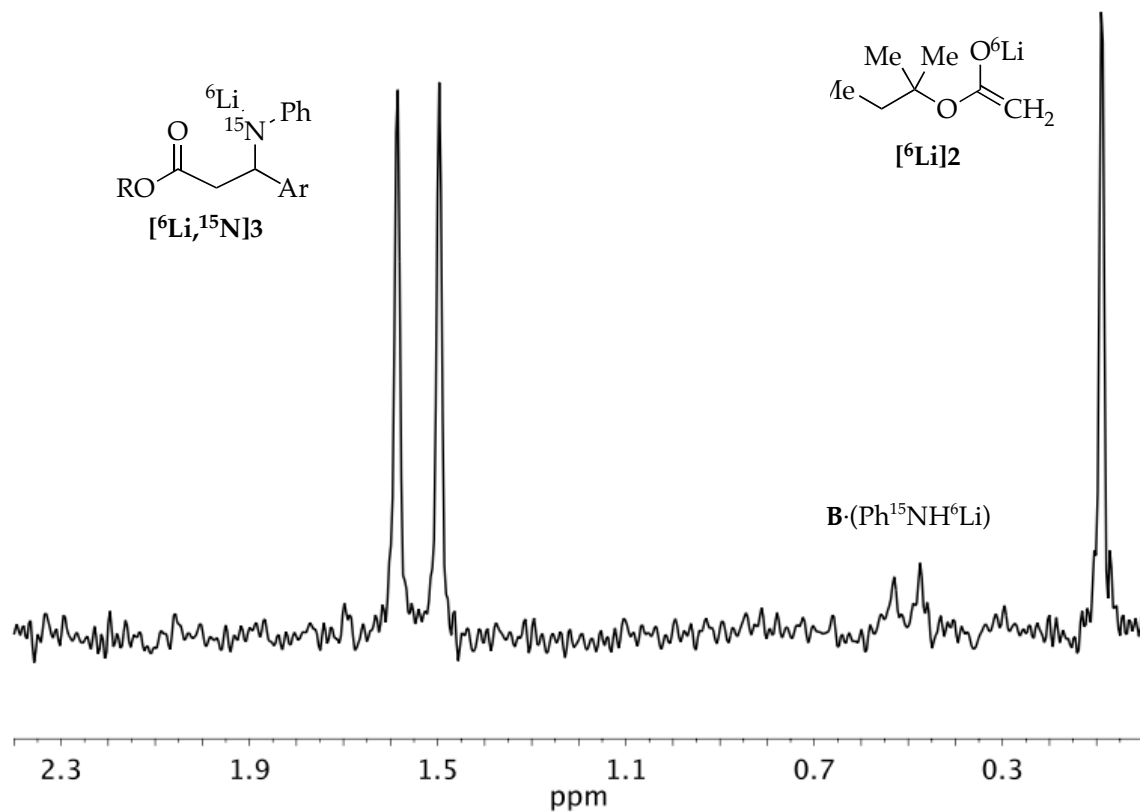




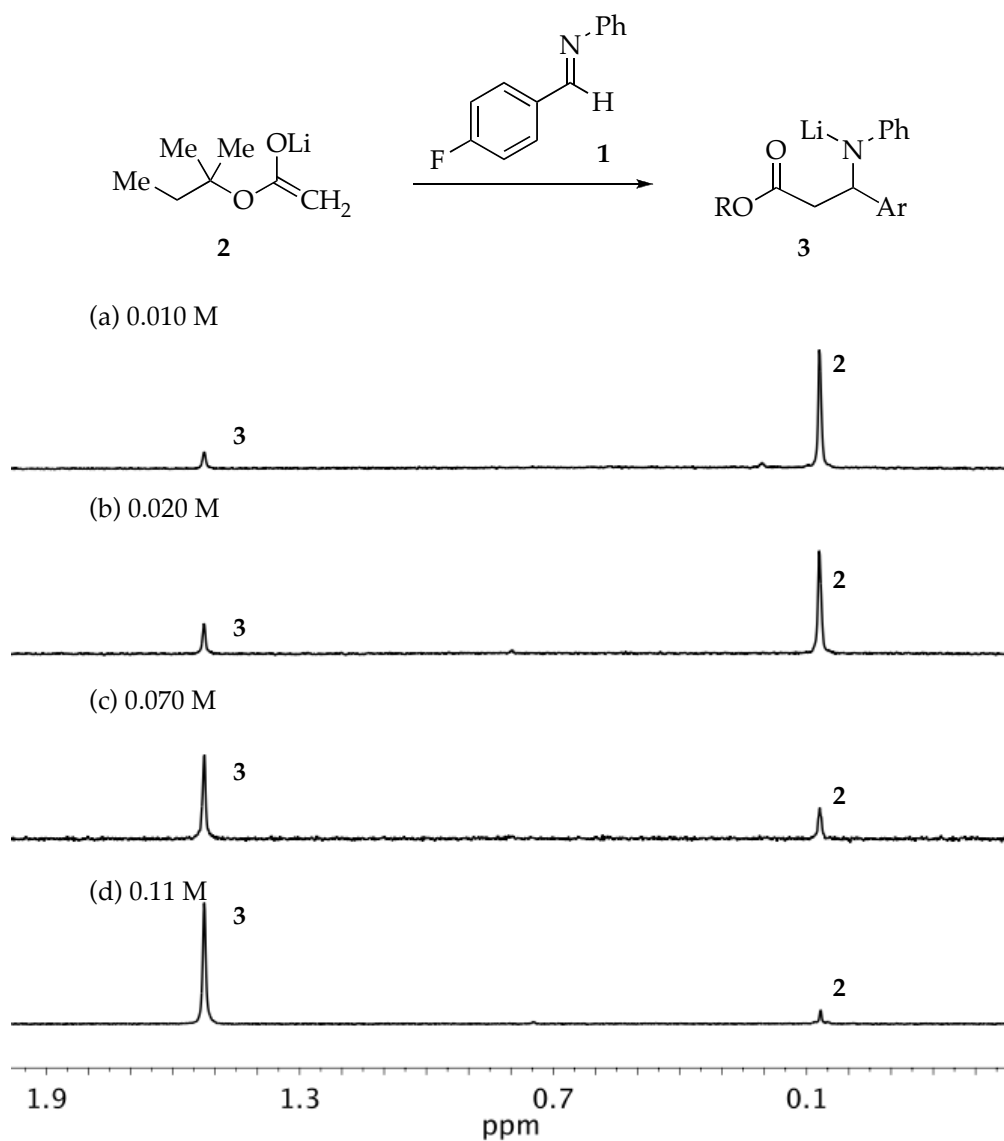
**Figure 6.**  $^{15}\text{N}$  NMR spectrum of a 0.10 M solution of  $[\text{}^6\text{Li}, \text{}^{15}\text{N}]\mathbf{3}$  in 0.60 M TMEDA/toluene at  $-60\text{ }^\circ\text{C}$  generated from adduct  $[\text{}^{15}\text{N}]\mathbf{4}$  and LiHMDS.



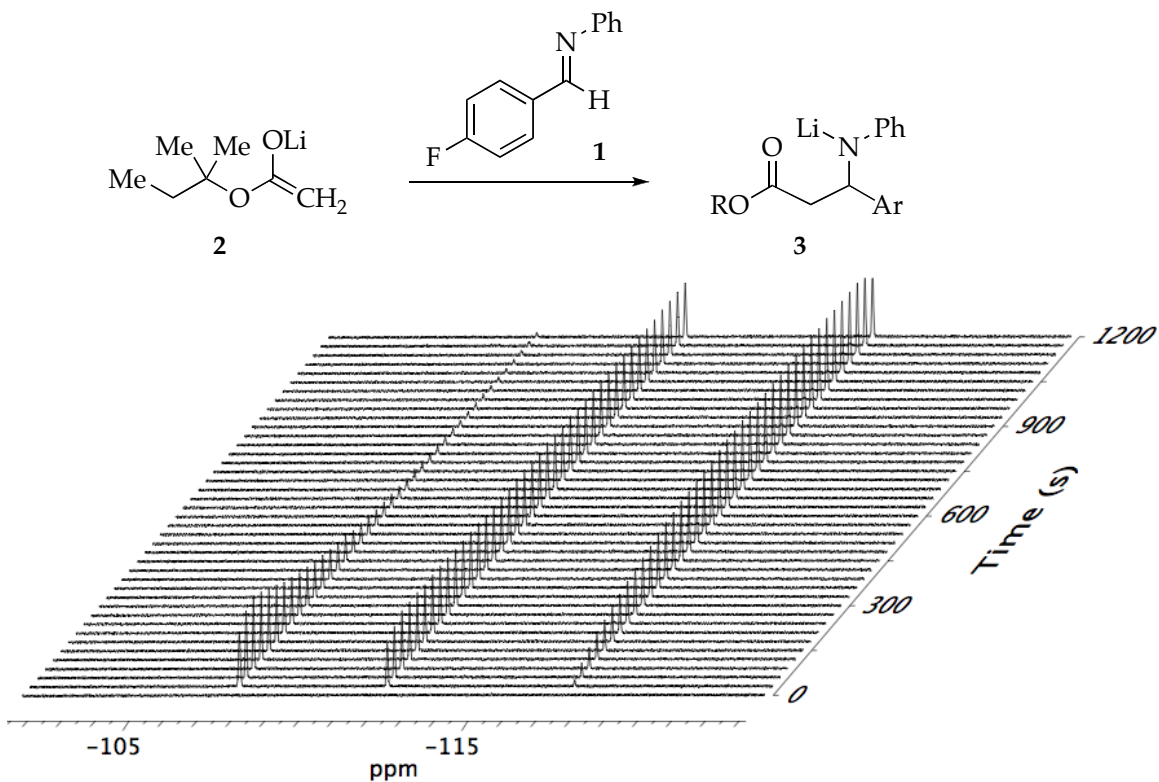
**Figure 7.**  $^{19}\text{F}$  NMR spectrum of a 0.10 M solution of  $[\text{Li}^6, \text{N}^{15}]3$  in 0.60 M TMEDA/toluene at  $-60\text{ }^\circ\text{C}$  generated from adduct  $[\text{N}^{15}]4$  and LiHMDS.



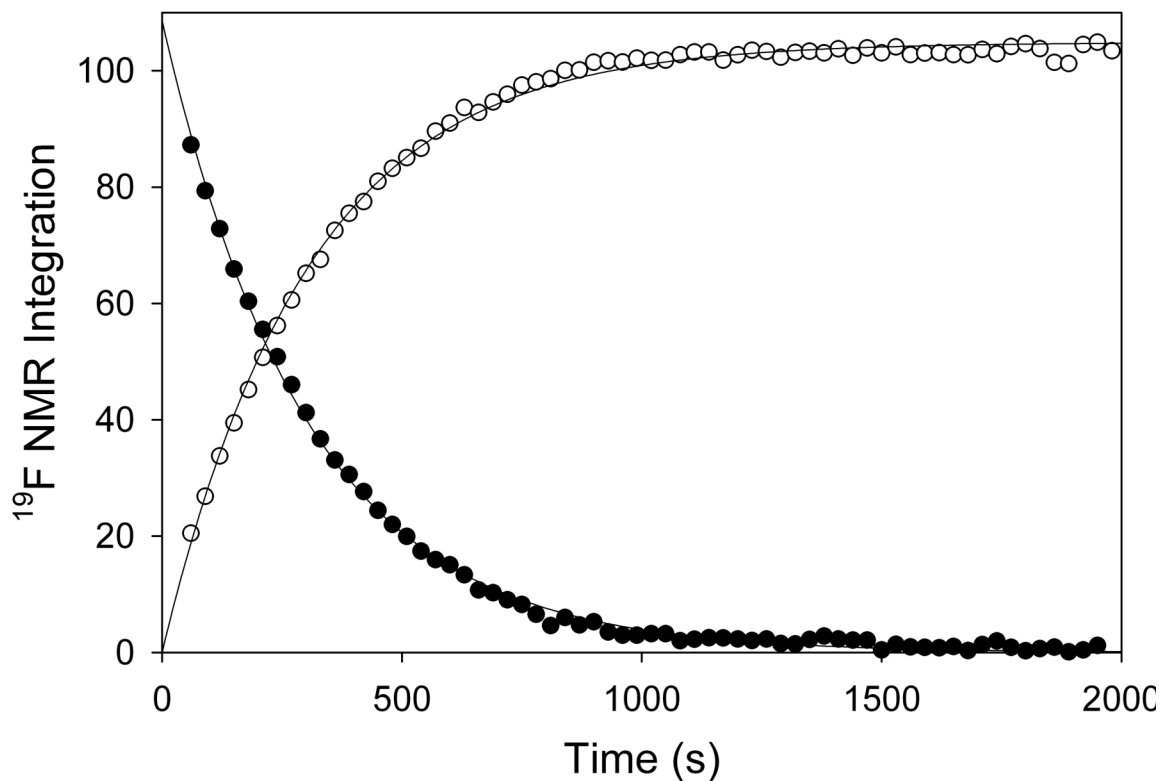
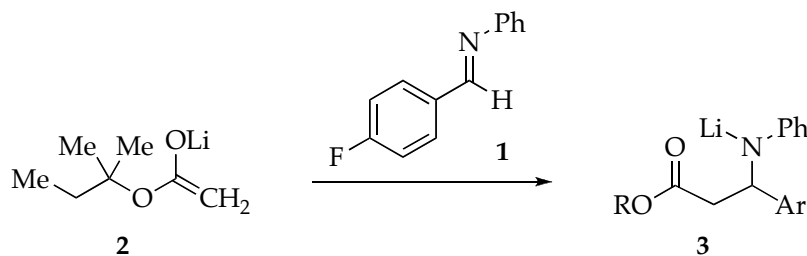
**Figure 8.**  ${}^6\text{Li}$  NMR spectrum of a solution of 0.050 M  $[\text{}^6\text{Li}, \text{}^{15}\text{N}]3$  and 0.050 M enolate  $[\text{}^6\text{Li}]2$  prepared using  $[\text{}^6\text{Li}]$ LDA in 0.60 M TMEDA/toluene at  $-60\text{ }^\circ\text{C}$ .



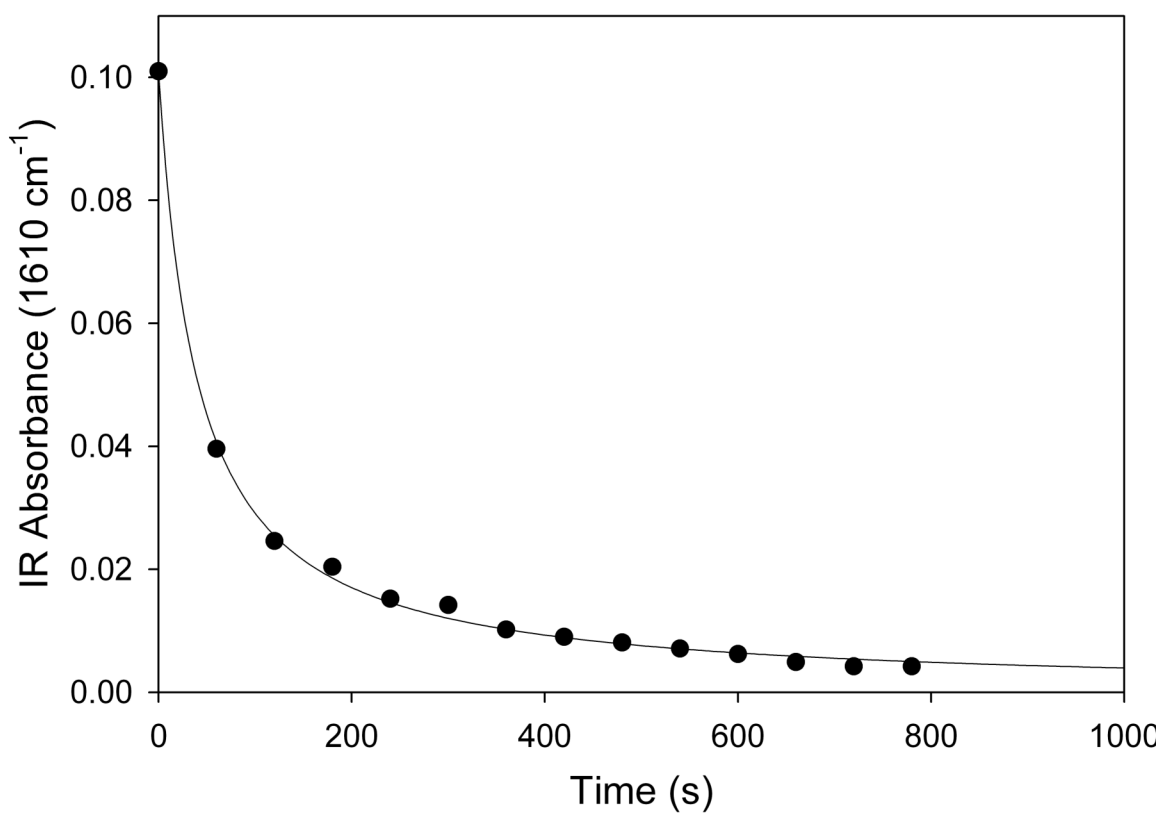
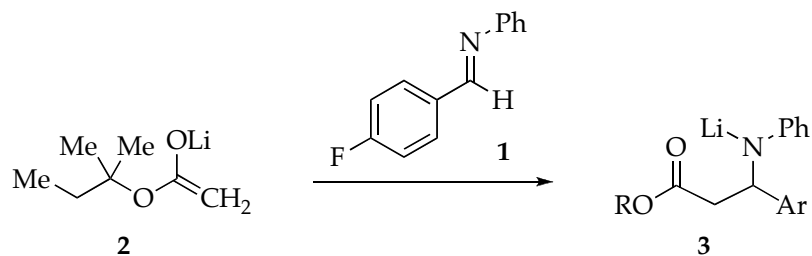
**Figure 9.** Representative  $^6\text{Li}$  NMR spectroscopic analysis of the condensation of the lithium enolate of *tert*-amyl acetate (**2**, 0.10 M) with the following concentrations of *N*-(4-fluorobenzylidene)-aniline (**1**): (a) 0.010 M, (b) 0.020 M, (c) 0.070 M, (d) 0.11 M) in 0.55 M TMEDA/toluene at  $-60^\circ\text{C}$ .



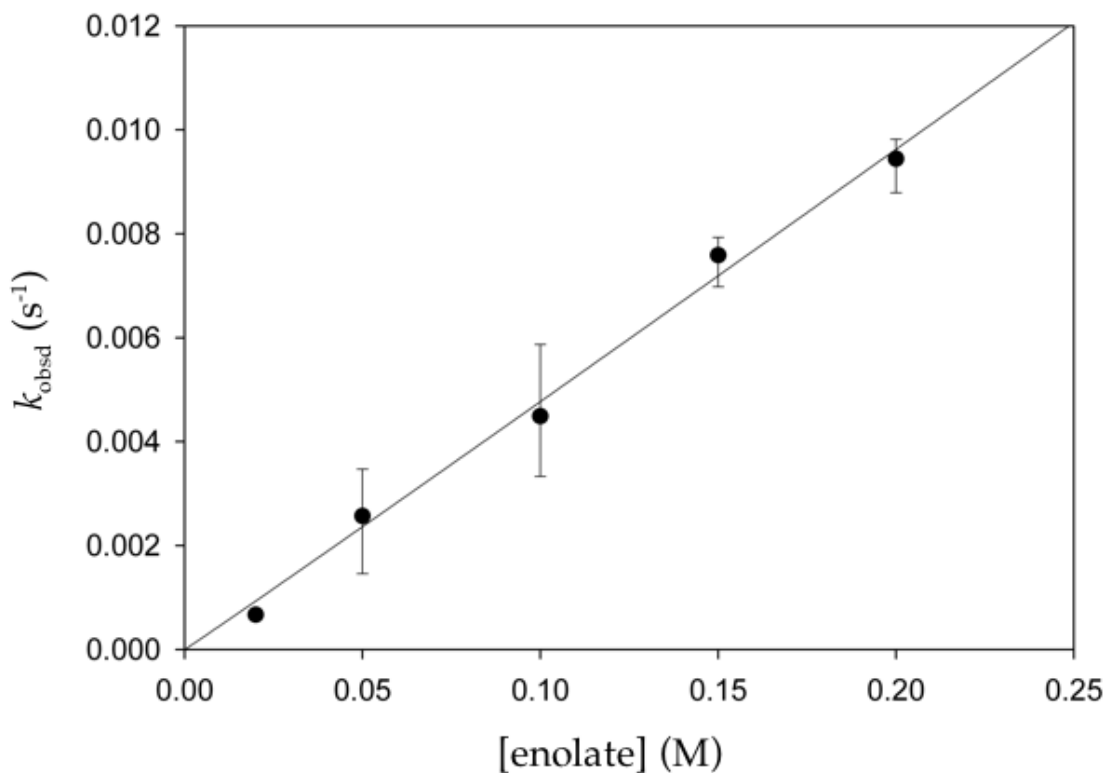
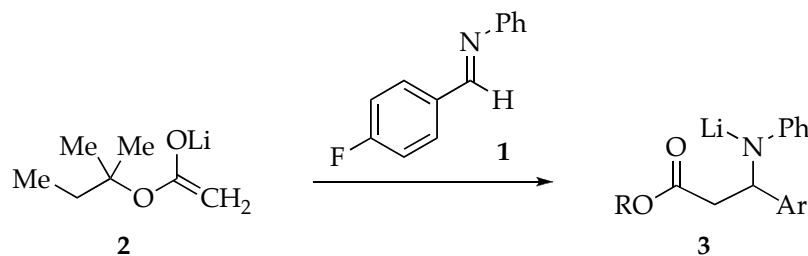
**Figure 10.** Representative  $^{19}\text{F}$  NMR spectroscopic analysis of the condensation of the lithium enolate of *tert*-amyl acetate (**2**, 0.10 M) with *N*-(4-fluorobenzylidene)-aniline (**1**, 0.005 M) in 0.55 M TMEDA/toluene at  $-60\text{ }^\circ\text{C}$ . The resonances correspond to **1** ( $\delta$  -107.4 ppm), **2** ( $\delta$  -117.2 ppm) and internal standard (fluorobenzene, 0.007 M,  $\delta$  -112.96 ppm).



**Figure 11.** Representative curve fitting for the condensation of the lithium enolate of *tert*-amyl acetate (**2**, 0.10 M) with *N*-(4-fluorobenzylidene)aniline (**1**, 0.005 M) in 0.55 M TMEDA/toluene at  $-60\text{ }^{\circ}\text{C}$ . Imine **1** is represented by the symbol  $\bullet$  and product **3** by  $\circ$ . The curves depict unweighted least-squares fits to  $y_1 = y_0 \cdot e^{-b \cdot t}$  ( $y_0 = 108.6 \pm 0.1$ ,  $b = 3.32 \pm 0.03 \times 10^{-3} \text{ s}^{-1}$ ) and  $y_{s3} = y_0 \cdot (1 - e^{-b \cdot t})$  ( $y_0 = 104.9 \pm 0.1$ ,  $b = 3.28 \pm 0.03 \times 10^{-3} \text{ s}^{-1}$ ).



**Figure 12.** Condensation of the lithium enolate of *tert*-amyl acetate (**2**, 0.10 M) with stoichiometric *N*-(4-fluorobenzylidene)aniline (**1**, 0.10 M) in 0.65 M TMEDA/toluene at -60 °C. The curve depicts and unweighted least-squares fit to  $y = [A]_0 / (1 + [A]_0 \cdot k \cdot t)$  ( $[A]_0 = 0.101 \pm 0.001$  M,  $k = 0.24 \pm 0.01$  M<sup>-1</sup> s<sup>-1</sup>).

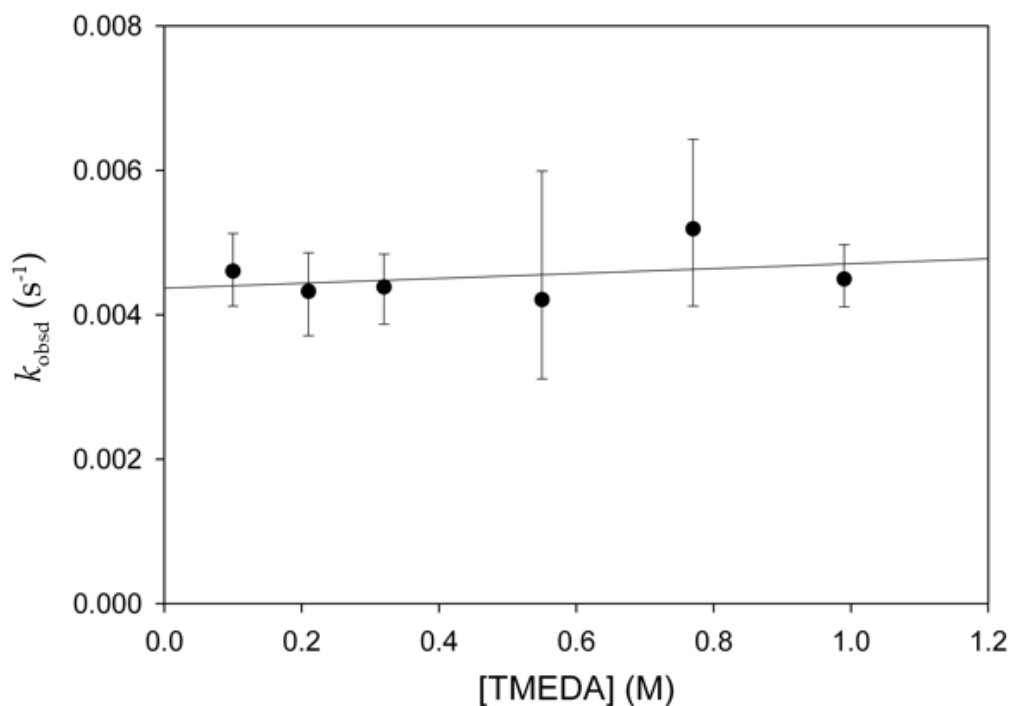


**Figure 13.** Plot of  $k_{\text{obsd}}$  versus [2] for the condensation of enolate 2 with *N*-(4-fluorobenzylidene)aniline (1, 0.005 M) in 0.60 M TMEDA/toluene at  $-60$  °C. The curve depicts the result of an unweighted least-squares fit to  $k_{\text{obsd}} = k \cdot [2]^b$  ( $k = 0.049 \pm 0.007$ ,  $b = 1.01 \pm 0.08$ ).

[2] (N)	$k_{\text{obsd}} 1 \times 10^3$ ( $\text{s}^{-1}$ )	$k_{\text{obsd}} 2 \times 10^3$ ( $\text{s}^{-1}$ )	$k_{\text{obsd}} \text{ avg} \times 10^3$ ( $\text{s}^{-1}$ )
0.020 <sup>a</sup>	0.69 ± 0.01	0.65 ± 0.05	0.67
0.050 <sup>a</sup>	3.40 ± 0.07	1.7 ± 0.3	2.6
0.10	3.36 ± 0.03	5.6 ± 0.2	4.5
0.15	7.87 ± 0.06	7.3 ± 0.3	7.6
0.20	9.7 ± 0.1	9.2 ± 0.4	9.4

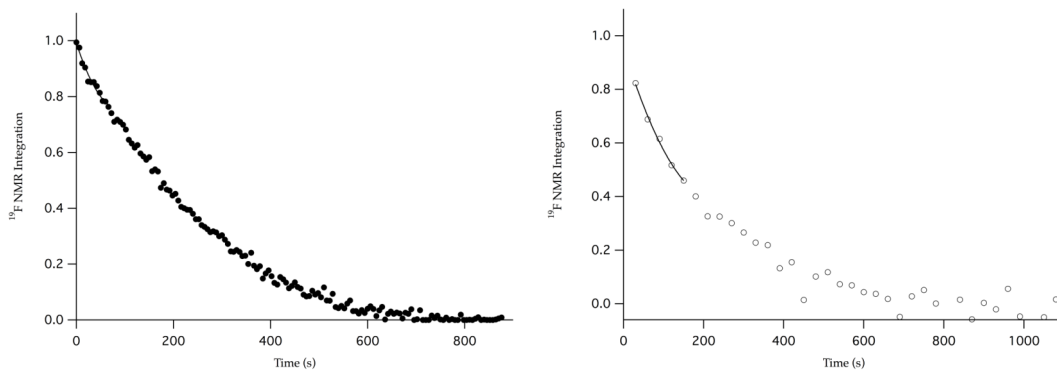
<sup>a</sup> [1]<sub>init</sub> = 0.001 M.



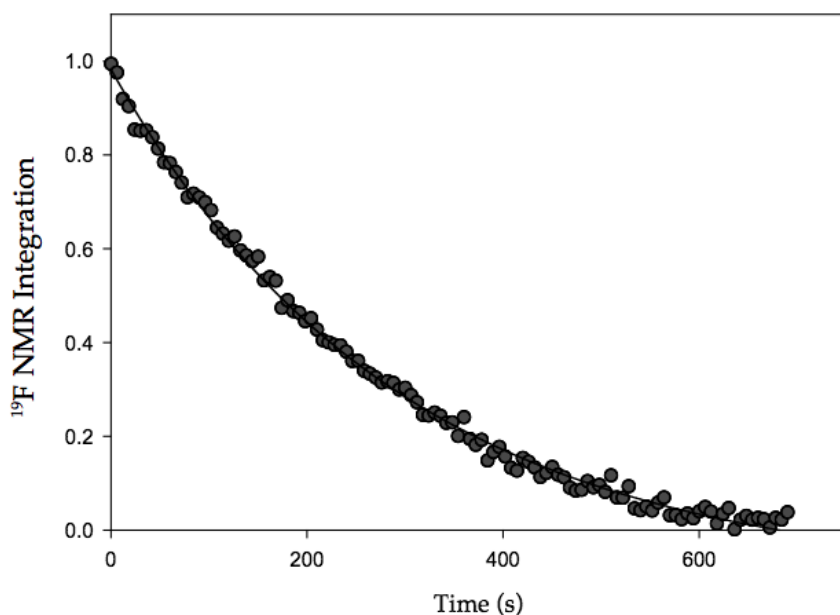


**Figure 14.** Plot of  $k_{\text{obsd}}$  versus excess [TMEDA] in toluene cosolvent for the condensation of the lithium enolate of *tert*-amyl acetate (**2**, 0.10 M) with *N*-(4-fluorobenzylidene)aniline (**1**, 0.005 M) at  $-60$  °C. The curve depicts the result of an unweighted least-squares fit to  $k_{\text{obsd}} = k + k' \cdot [\text{TMEDA}]_{\text{free}}$  ( $k = 0.0044 \pm 0.3$ ,  $k' = 0.3 \pm 0.5$ ).

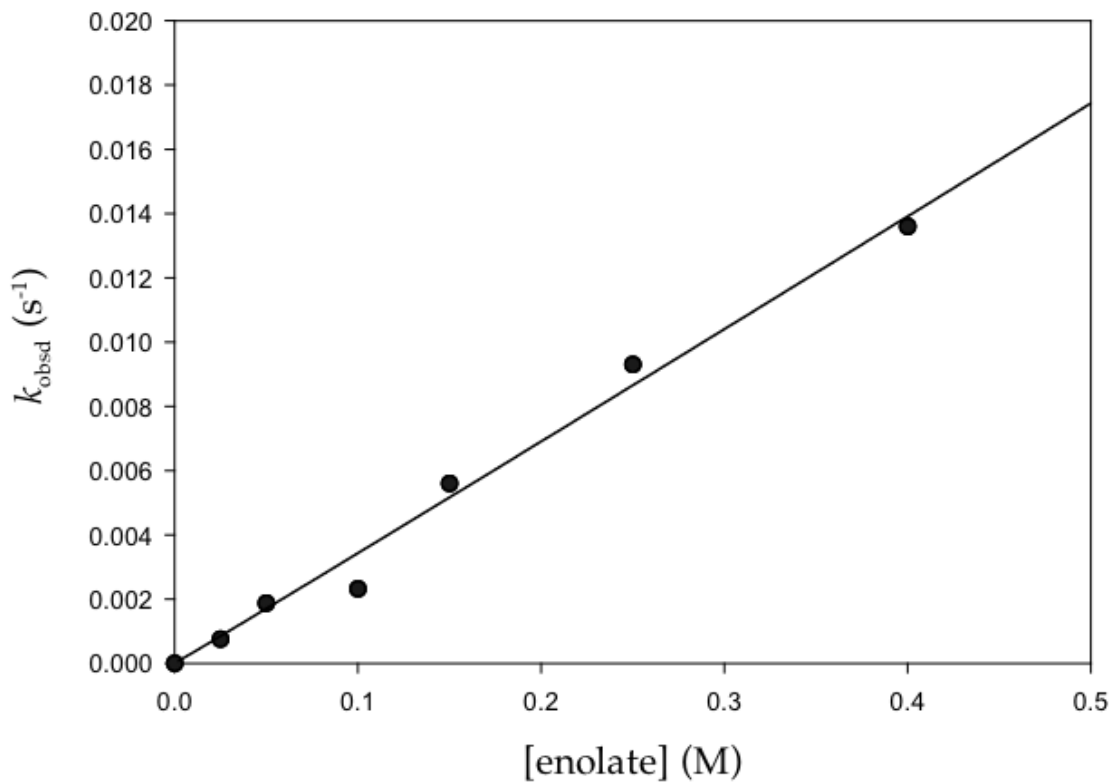
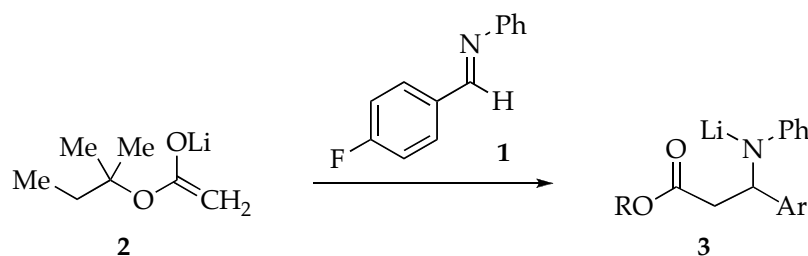
$[\text{TMEDA}]_{\text{free}}$ (M)	$k_{\text{obsd}} 1 \times 10^3$ ( $\text{s}^{-1}$ )	$k_{\text{obsd}} 2 \times 10^3$ ( $\text{s}^{-1}$ )	$k_{\text{obsd}} \text{ avg} \times 10^3$ ( $\text{s}^{-1}$ )
0.10	$4.18 \pm 0.06$	$5.0 \pm 0.1$	4.6
0.21	$4.80 \pm 0.06$	$3.9 \pm 0.1$	4.3
0.32	$4.80 \pm 0.04$	$4.0 \pm 0.1$	4.4
0.55	$3.36 \pm 0.03$	$3.2 \pm 0.1$	
0.55	$5.7 \pm 0.3$	$4.6 \pm 0.1$	4.2
0.77	$4.2 \pm 0.1$	$6.2 \pm 0.3$	5.2
0.99	$4.16 \pm 0.05$	$4.8 \pm 0.1$	4.5



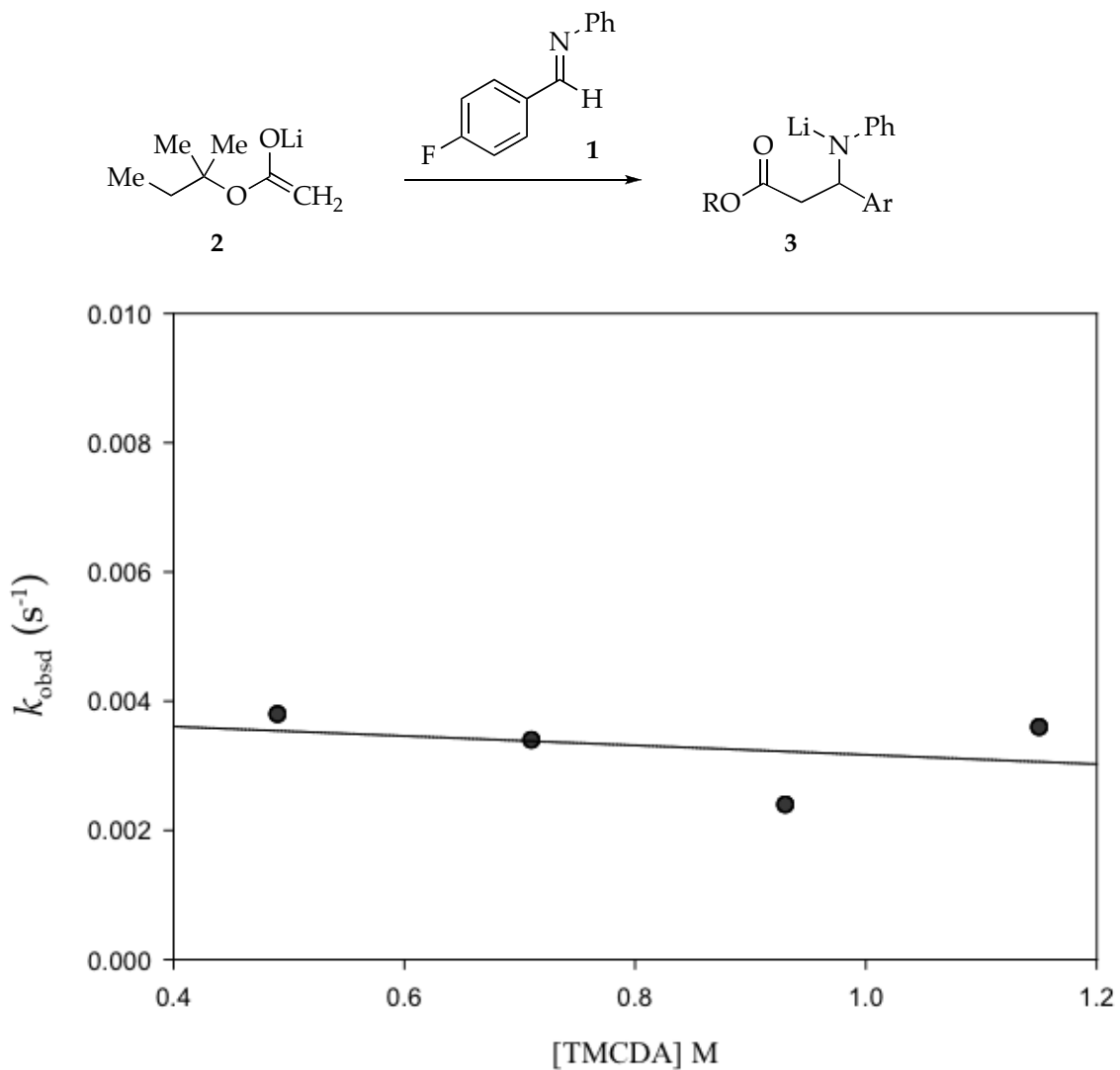
**Figure 15.** Initial rate curve fitting for the condensation of the lithium enolate of *tert*-amyl acetate (**2**, 0.10 M) with *N*-(4-fluorobenzylidene)aniline (**1**, 0.005 M) in 0.70 M TMCDA/toluene at -60 °C (left) and in 0.70 M TMEDA/toluene at -60 °C (right). The curves depict unweighted least-squares fits to  $y_1 = y_0 + bx + cx^2$ ;  $y_0 = 0.95543 \pm 0.0299$  M,  $b = -0.0048636 \pm 0.00076$  M<sup>-1</sup> s<sup>-1</sup>,  $c = 1.0381e^{-5} \pm 4.14e^{-6}$  (left);  $y_0 = 0.99133 \pm 0.0106$  M,  $b = -0.0053595 \pm 0.000743$  M<sup>-1</sup> s<sup>-1</sup>,  $c = 3.0665e^{-5} \pm 1.09e^{-5}$  (right) where  $b = k_{\text{obsd}} \cdot (k_{\text{TMCDA}} / k_{\text{TMEDA}}) = (-0.0048636 / -0.0053595) = 0.91$ .



**Figure 16.** Representative curve fitting for the condensation of the lithium enolate of *tert*-amyl acetate (**2**, 0.10 M) with *N*-(4-fluorobenzylidene)aniline (**1**, 0.005 M) with 7 equiv TMCDA at -60 °C. Imine **1** is represented by the symbol •. The curve depicts unweighted least-squares fits to  $y_1 = y_0 \cdot (1 + e^{-bt})$ ;  $y_0 = 1.0$  M,  $b = 3.4 \times 10^{-3}$  s<sup>-1</sup>.

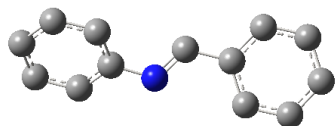
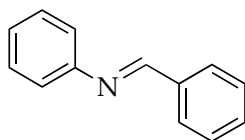


**Figure 17.** Plot of  $k_{\text{obsd}}$  versus [2] for the condensation of enolate **2** with *N*-(4-fluorobenzylidene)aniline (**1**, 0.005 M) in 7 equiv TMCDA/toluene at  $-60\text{ }^{\circ}\text{C}$ . The curve depicts the result of an unweighted least-squares fit to  $k_{\text{obsd}} = k \cdot [\mathbf{2}]^b$ ;  $b = 1.01$ .



**Figure 18.** Plot of  $k_{\text{obsd}}$  versus [TMCDA] in toluene cosolvent for the condensation of the lithium enolate of *tert*-amyl acetate (2, 0.10 M) with *N*-(4-fluorobenzylidene)aniline (1, 0.005 M) at  $-60\text{ }^{\circ}\text{C}$  showing a zero-order dependency on [TMCDA].

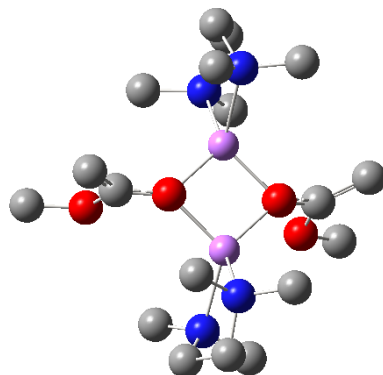
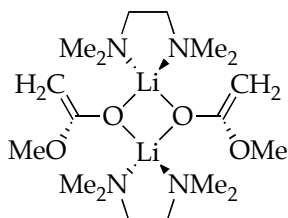
**Table 1: Thermally corrected MP2 energies for ground and transition structures.**



**1**  
 $G = -554.7569897$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	0.401497	0.403579	-0.169238	H	0.095103	1.404539	-0.510148
N	-0.456713	-0.503666	0.115513	C	1.849830	0.181027	-0.082378
C	-1.832073	-0.214580	0.068027	C	2.728064	1.219922	-0.426913
C	-2.695626	-1.228360	-0.379684	C	4.108208	1.036109	-0.352880
C	-4.068399	-1.007563	-0.447704	C	4.624318	-0.191253	0.065761
C	-4.607288	0.215864	-0.039052	C	3.755773	-1.233762	0.410433
C	-3.759028	1.216412	0.439297	C	2.379297	-1.051601	0.338961
C	-2.381414	1.008509	0.492809	H	1.690868	-1.848009	0.602599
H	-1.729703	1.777881	0.897430	H	4.158372	-2.189196	0.736249
H	-4.171807	2.162086	0.781442	H	5.699605	-0.337749	0.123990
H	-5.680399	0.381405	-0.077523	H	4.778854	1.847696	-0.621603
H	-4.722393	-1.796406	-0.810126	H	2.322945	2.175220	-0.753984
H	-2.263401	-2.177633	-0.681557				

**Table 1(continued)**

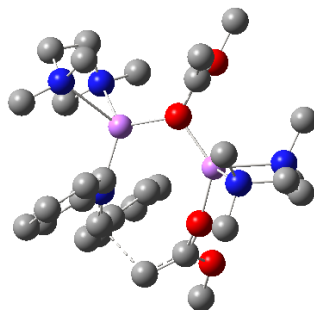
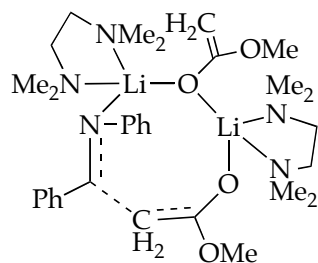


**2**  
 $G = -1241.537100$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	0.225739	4.291968	-1.490664	C	-2.803888	-0.975202	-2.102770
O	0.300275	2.958600	-1.019421	H	-2.935270	-1.883451	-1.508943
C	-0.253160	2.672353	0.233120	H	-3.594874	-0.941031	-2.874115
O	-0.084969	1.422097	0.541140	H	-1.826932	-1.046359	-2.586590
Li	-1.271903	-0.019384	0.238451	H	-4.964850	0.072159	-1.053090
O	0.080946	-1.306950	-0.003128	H	-4.171872	1.310862	-0.077833
Li	1.273392	0.155506	0.246022	H	-3.967060	-1.710500	0.388391
C	0.081443	-2.520899	-0.460156	H	-5.003784	-0.606666	1.295094
C	-0.112700	-3.664480	0.250352	C	-2.634305	-1.612418	2.486104
H	-0.097876	-4.652508	-0.188230	H	-2.405893	-2.475151	1.854466
H	-0.263244	-3.590755	1.319959	H	-1.761820	-1.413895	3.116001
O	0.319164	-2.537706	-1.838521	H	-3.487842	-1.858940	3.143537
C	0.348592	-3.791793	-2.496844	C	-3.093929	0.752815	2.478818
H	0.546206	-3.582851	-3.551681	H	-2.210791	0.900186	3.106218
H	1.142203	-4.438973	-2.099610	H	-3.201244	1.645191	1.857953
H	-0.610735	-4.318476	-2.404364	H	-3.981549	0.659627	3.131316
C	-0.884740	3.619711	0.976143	N	2.688312	-0.314029	1.874981
H	-0.986110	4.651533	0.670029	C	4.017509	-0.159257	1.260684
H	-1.252096	3.346044	1.957159	C	3.999510	-0.475274	-0.239298
H	0.726099	4.990757	-0.806786	N	3.045137	0.368386	-0.976714
H	0.731198	4.308099	-2.460225	C	2.779199	-0.179056	-2.313972
H	-0.815309	4.617744	-1.621268	H	2.073135	0.477627	-2.830637
N	-2.898243	-0.439517	1.645067	H	3.698405	-0.251480	-2.923779
C	-4.043752	-0.680289	0.750937	H	2.315387	-1.164446	-2.227009
C	-4.069331	0.282872	-0.439631	C	3.500507	1.759497	-1.088896
N	-2.835187	0.212269	-1.238721	H	3.682485	2.187549	-0.099953
C	-2.648206	1.428353	-2.039790	H	4.429567	1.842681	-1.682249
H	-1.689354	1.372532	-2.561482	H	2.711644	2.350971	-1.557294
H	-3.452410	1.563748	-2.785773	H	5.025323	-0.375653	-0.642033
H	-2.620498	2.299706	-1.379498	H	3.699640	-1.518317	-0.389889

Atom	X	Y	Z
H	4.343193	0.874123	1.413850
H	4.770657	-0.798792	1.754903
C	2.523065	0.553378	3.045329
H	2.665227	1.598876	2.756369
H	1.504216	0.448361	3.429122
H	3.230584	0.309061	3.858613
C	2.416070	-1.711402	2.233991
H	1.394022	-1.794276	2.610215
H	2.481828	-2.357309	1.356035
H	3.116730	-2.079319	3.006079

**Table 1 (continued)**



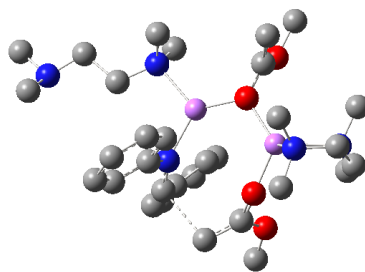
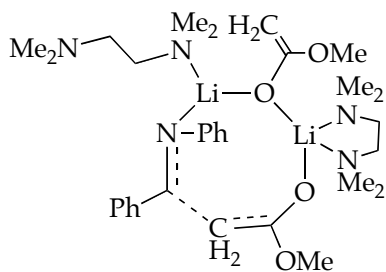
**5a**  
 $G = -1796.284042$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.820237	4.901310	0.962154	H	2.305937	1.966373	2.228094
O	-1.353819	3.618846	0.649713	N	2.484331	-0.718293	-2.319942
C	-0.984327	2.517143	1.391500	C	2.725818	-2.146459	-2.598819
O	-1.560698	1.460861	1.051331	C	3.369795	-2.901360	-1.438294
Li	-2.007465	-0.054322	0.042895	N	2.559965	-2.886434	-0.210122
O	-0.711084	-1.146583	-0.911199	C	3.421164	-3.031398	0.969977
Li	1.158889	-0.818042	-0.517848	H	2.809376	-3.026103	1.873680
N	1.449803	0.374706	1.158906	H	4.004773	-3.970600	0.945297
C	1.471696	-0.445685	2.302725	H	4.117938	-2.189820	1.027477
C	0.514606	-1.478423	2.405686	C	1.563318	-3.964606	-0.226039
C	0.495612	-2.341912	3.500533	H	2.040583	-4.961947	-0.275442
C	1.430200	-2.207860	4.531265	H	0.964330	-3.911815	0.686754
C	2.388912	-1.195999	4.441671	H	0.881897	-3.855044	-1.072881
C	2.413509	-0.330401	3.348984	H	3.578484	-3.936163	-1.766523
H	3.192671	0.424636	3.292362	H	4.342707	-2.455442	-1.212045
H	3.134541	-1.084390	5.225878	H	1.758761	-2.596612	-2.850808
H	1.414214	-2.880405	5.384472	H	3.376806	-2.263057	-3.487239
H	-0.258349	-3.125011	3.550970	C	3.730575	0.002831	-2.021458
H	-0.214240	-1.583672	1.607282	H	3.508960	1.066870	-1.919080
C	1.726883	1.666423	1.351893	H	4.484757	-0.126463	-2.819530
C	1.940680	2.572377	0.191504	H	4.157433	-0.337255	-1.075283
C	1.163125	2.495274	-0.975124	C	1.836189	-0.111681	-3.493747
C	1.376939	3.385303	-2.028256	H	1.674347	0.951579	-3.306141
C	2.379821	4.355619	-1.946618	H	2.459723	-0.213931	-4.401041
C	3.163455	4.436899	-0.793809	H	0.866756	-0.585096	-3.658948
C	2.939344	3.556653	0.265710	C	-1.203466	-1.972176	-1.792448
H	3.547569	3.629003	1.165166	C	-1.681013	-3.225935	-1.567065
H	3.948136	5.185532	-0.717869	H	-2.085326	-3.861356	-2.342714
H	2.544228	5.044597	-2.770958	H	-1.638818	-3.624241	-0.562040
H	0.750084	3.326394	-2.914710	O	-1.198782	-1.412085	-3.072621
H	0.370899	1.756189	-1.036644	C	-1.653634	-2.206916	-4.155616



Atom	X	Y	Z	Atom	X	Y	Z
H	-1.524167	-1.602157	-5.056946	H	-5.770270	0.923512	-0.346627
H	-1.070114	-3.132260	-4.249445	H	-4.448823	1.472750	0.697402
H	-2.713739	-2.470697	-4.045831	C	-3.537597	1.994158	-1.587020
N	-3.786106	0.635394	-1.085164	H	-2.809108	1.945009	-2.402489
C	-4.757154	0.669844	0.020821	H	-4.459244	2.466355	-1.974811
C	-4.831182	-0.651328	0.789449	H	-3.115995	2.610069	-0.790765
N	-3.563040	-1.000214	1.456218	C	-4.235667	-0.222283	-2.187325
C	-3.431857	-0.301330	2.743111	H	-5.207232	0.108971	-2.599146
H	-2.463425	-0.542557	3.188654	H	-3.484735	-0.194203	-2.979394
H	-4.233716	-0.594520	3.445781	H	-4.324717	-1.260669	-1.859896
H	-3.459796	0.778312	2.591868	C	0.044976	2.593120	2.354382
C	-3.475694	-2.448603	1.671671	H	0.400561	3.559417	2.695247
H	-2.524272	-2.684189	2.158213	H	0.022121	1.817068	3.110975
H	-4.292130	-2.828880	2.312949	H	0.260393	4.940525	0.789757
H	-3.505706	-2.966432	0.709687	H	-1.317093	5.603420	0.288637
H	-5.083634	-1.462004	0.099456	H	-1.036536	5.181932	2.000382
H	-5.660414	-0.594469	1.518227				

**Table 1 (continued)**

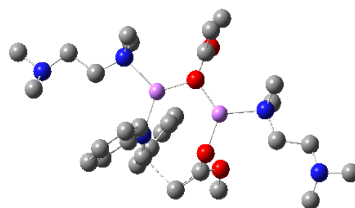
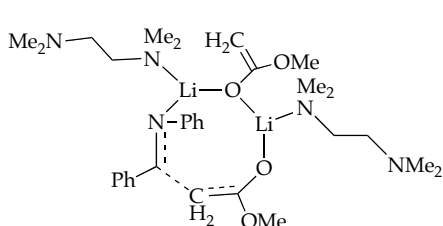


**5b**  
 $G = -1796.271055$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	1.777519	4.368765	-1.567035	C	-1.221948	-0.841642	-2.146086
O	2.137676	3.064398	-1.127635	C	-2.125845	-0.779605	-3.229578
C	1.652533	1.957719	-1.797806	C	-2.328020	-1.881582	-4.059506
O	2.087913	0.866459	-1.358473	C	-1.648463	-3.081124	-3.837482
Li	2.532703	-0.323298	0.003748	C	-0.758518	-3.163021	-2.763359
O	1.138490	-0.939824	1.180018	C	-0.547454	-2.064645	-1.932415
Li	-0.555985	-0.483629	0.594987	H	0.165719	-2.129120	-1.113512
N	-2.281004	-1.048467	1.694784	H	-0.219596	-4.088444	-2.572770
C	-2.216370	-0.312675	2.967298	H	-1.813092	-3.937010	-4.485981
H	-2.353479	0.756307	2.775233	H	-3.034016	-1.802835	-4.883171
H	-2.977329	-0.639994	3.694775	H	-2.695542	0.126902	-3.410796
H	-1.227922	-0.454577	3.414157	C	-1.170071	1.453040	-1.608024
C	-2.150613	-2.498559	1.918653	C	-1.258986	2.525239	-0.586975
H	-1.169818	-2.711950	2.356456	C	-0.539200	2.481868	0.620330
H	-2.927917	-2.898841	2.589457	C	-0.690629	3.488750	1.573588
H	-2.220213	-3.019623	0.957939	C	-1.560590	4.557817	1.342816
C	-3.465336	-0.695385	0.880510	C	-2.272746	4.617473	0.143056
H	-3.431992	0.382923	0.693818	C	-2.119965	3.611945	-0.811536
H	-3.335688	-1.189322	-0.087065	H	-2.682137	3.660244	-1.741727
C	-4.843887	-1.037470	1.475762	H	-2.951936	5.444370	-0.048271
N	-5.933649	-0.500464	0.657484	H	-1.677234	5.339968	2.088312
C	-6.092035	-1.210136	-0.607658	H	-0.115678	3.441915	2.494852
H	-6.900940	-0.747121	-1.183035	H	0.181766	1.688546	0.795470
H	-5.180813	-1.145325	-1.208096	H	-1.700131	1.684462	-2.532175
H	-6.339717	-2.282565	-0.472388	C	1.387108	-1.483128	2.341732
C	-7.190512	-0.484983	1.394718	C	1.621896	-2.798280	2.590534
H	-7.970429	-0.021627	0.780215	H	1.826161	-3.192401	3.576388
H	-7.542912	-1.495359	1.684853	H	1.590301	-3.496780	1.763989
H	-7.079660	0.110789	2.307232	O	1.373507	-0.522934	3.350695
H	-4.948627	-2.131516	1.619039	C	1.615145	-0.948856	4.682416
H	-4.928773	-0.579744	2.467993	H	1.558441	-0.053538	5.306300
N	-0.996463	0.196693	-1.228799	H	0.861822	-1.674805	5.015877

Atom	X	Y	Z	Atom	X	Y	Z
H	2.609701	-1.402338	4.784994	C	4.493918	1.772536	0.995030
N	3.792988	-1.855288	-1.065855	H	5.499803	2.133476	1.278305
C	3.353992	-3.246441	-0.913268	H	4.204184	2.201941	0.034296
H	3.287835	-3.496750	0.148907	H	3.778374	2.122346	1.745050
H	4.036327	-3.961006	-1.409220	C	4.680994	-0.266621	2.252224
H	2.360360	-3.361336	-1.356453	H	5.697340	-0.034204	2.620948
C	3.785713	-1.482484	-2.487543	H	3.947493	0.141929	2.951165
H	4.066348	-0.434854	-2.606699	H	4.547950	-1.350797	2.238390
H	4.475438	-2.114485	-3.076749	H	6.429977	-0.103180	0.271290
H	2.773660	-1.591499	-2.884324	C	0.673646	2.084360	-2.795692
C	5.123120	-1.657504	-0.463240	H	0.430225	3.049131	-3.224729
H	5.183989	-2.286268	0.430440	H	0.552081	1.227929	-3.447903
H	5.925567	-2.000398	-1.141897	H	0.704183	4.551938	-1.448739
C	5.385085	-0.198636	-0.081007	H	2.332205	5.063576	-0.931928
H	5.289157	0.435564	-0.968335	H	2.061939	4.529941	-2.614536
N	4.435204	0.306239	0.923608				

**Table 1 (continued)**

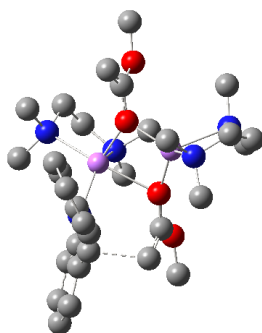
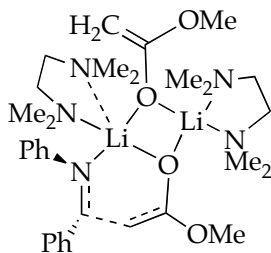


**5c**  
 $G = -1796.254494$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.524718	-2.642382	2.435494	C	1.759408	-1.626556	-1.579551
O	-2.442079	-1.731727	1.339731	C	2.686996	-2.673175	-1.783023
C	-1.672640	-2.048717	0.239169	C	3.153303	-2.983240	-3.060063
O	-1.752737	-1.218347	-0.695149	C	2.723774	-2.259862	-4.175419
Li	-1.907580	0.611585	-0.597665	C	1.812181	-1.217311	-3.992151
O	-0.434576	1.734850	-0.387983	C	1.335900	-0.907698	-2.719534
Li	1.159014	0.767335	-0.269159	H	0.591143	-0.124944	-2.593794
N	3.012282	1.797240	-0.157710	H	1.455135	-0.649019	-4.847898
C	3.003629	2.483631	1.143486	H	3.092444	-2.504521	-5.167624
H	3.021233	1.739717	1.946471	H	3.869618	-3.792878	-3.181704
H	3.858399	3.166173	1.279040	H	3.069204	-3.227904	-0.930659
H	2.082507	3.066276	1.237436	C	1.091783	-2.139704	0.619279
C	3.023205	2.768790	-1.264657	C	0.973663	-1.718956	2.044180
H	2.114350	3.377641	-1.219119	C	0.443305	-0.475423	2.428549
H	3.895683	3.441448	-1.235591	C	0.374400	-0.116488	3.775387
H	3.033708	2.229296	-2.217625	C	0.830946	-0.989002	4.766246
C	4.085820	0.783518	-0.268748	C	1.356369	-2.229290	4.397705
H	3.946954	0.063446	0.544395	C	1.424366	-2.587678	3.051217
H	3.910294	0.244269	-1.203921	H	1.839850	-3.553594	2.771164
C	5.535648	1.299900	-0.212702	H	1.719763	-2.916353	5.157793
N	6.496424	0.203105	-0.079283	H	0.777376	-0.705866	5.814181
C	6.580313	-0.624561	-1.278573	H	-0.044421	0.849110	4.046938
H	7.305508	-1.428228	-1.111300	H	0.053012	0.211109	1.683353
H	5.616491	-1.090474	-1.499762	H	1.561447	-3.119891	0.511797
H	6.903120	-0.055249	-2.173766	C	-0.542157	3.018153	-0.144815
C	7.813986	0.701136	0.293573	C	-0.586314	4.013515	-1.065581
H	8.494376	-0.143314	0.449908	H	-0.674333	5.060015	-0.808237
H	8.266462	1.364314	-0.471124	H	-0.528985	3.751885	-2.115031
H	7.747988	1.262045	1.232377	O	-0.608139	3.251334	1.224167
H	5.759986	1.927701	-1.098543	C	-0.738111	4.593799	1.667841
H	5.656023	1.941439	0.667763	H	-0.776493	4.553673	2.758847
N	1.294578	-1.213141	-0.321845	H	0.118259	5.205141	1.354760

Atom	X	Y	Z	Atom	X	Y	Z
H	-1.658619	5.054038	1.286055	C	-8.472497	-0.235282	-1.475620
N	-3.887594	1.331672	-0.504692	H	-8.970667	-0.073591	-0.498398
C	-3.988767	1.684529	0.921585	H	-8.553652	0.691259	-2.054527
H	-3.864638	0.778598	1.523191	H	-9.024118	-1.017714	-2.008400
H	-4.951026	2.154271	1.181622	C	-6.950376	-1.902190	-0.667074
H	-3.184540	2.381238	1.179633	H	-7.300823	-1.863777	0.384486
C	-4.063090	2.516135	-1.358242	H	-7.546988	-2.654004	-1.194560
H	-4.010197	2.214527	-2.409804	H	-5.912064	-2.244137	-0.668293
H	-5.024403	3.030046	-1.193395	H	-6.549238	0.553921	0.348848
H	-3.252485	3.225679	-1.163815	C	-0.765445	-3.129327	0.256140
C	-4.771200	0.204061	-0.880343	H	-0.841281	-3.896696	1.018817
H	-4.572185	-0.037919	-1.930652	H	-0.468437	-3.479479	-0.726245
H	-4.445697	-0.654091	-0.286684	H	-1.563703	-2.743306	2.948833
C	-6.285405	0.438719	-0.722176	H	-3.257550	-2.215342	3.123516
H	-6.557472	1.378456	-1.216326	H	-2.870553	-3.628254	2.102561
N	-7.072756	-0.621175	-1.353915				

**Table 1 (continued)**

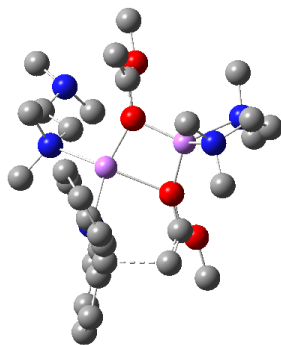
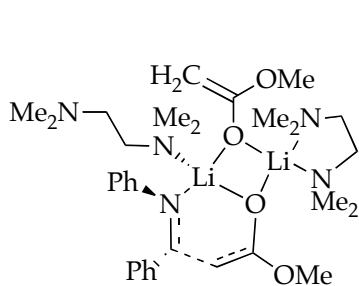


**5d**  
 $G = -1796.279143$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.688979	-0.758387	-3.567899	N	-1.234385	-1.476098	1.085363
O	-1.637032	-0.174186	-2.798865	C	-0.295681	-2.322623	1.695437
C	-0.898049	-0.956613	-1.952535	C	0.474027	-1.793509	2.757003
O	0.033073	-0.345279	-1.370319	C	1.393002	-2.564242	3.460041
Li	1.850090	-0.122591	-0.885426	C	1.601401	-3.907326	3.127402
O	1.547261	0.847057	0.698286	C	0.873120	-4.448750	2.068447
Li	-0.324437	0.463193	0.817734	C	-0.051375	-3.678905	1.359096
N	-1.135045	2.060380	2.379443	H	-0.591345	-4.154807	0.548082
C	-0.846892	3.419786	1.875138	H	1.020732	-5.488631	1.783787
C	-1.681875	3.877370	0.676164	H	2.314427	-4.513540	3.679190
N	-1.587930	3.019391	-0.503640	H	1.948607	-2.111661	4.278116
C	-2.662869	3.303612	-1.449530	H	0.325413	-0.756473	3.032371
H	-2.588968	4.318209	-1.889164	C	-2.117909	-2.060773	0.260545
H	-2.630503	2.571400	-2.261848	C	-3.429605	-1.425751	-0.058627
H	-3.634393	3.224162	-0.951460	C	-3.636344	-0.041398	-0.146520
C	-0.298138	3.145380	-1.183663	C	-4.905595	0.465119	-0.432549
H	0.524286	2.904146	-0.509167	C	-5.989374	-0.390626	-0.639646
H	-0.271849	2.431467	-2.010544	C	-5.794302	-1.770366	-0.561268
H	-0.144483	4.168153	-1.584852	C	-4.527742	-2.276436	-0.273880
H	-2.736717	3.930527	0.967209	H	-4.383191	-3.352820	-0.206272
H	-1.377290	4.919333	0.446888	H	-6.627132	-2.451894	-0.715362
H	-1.018104	4.162657	2.679499	H	-6.973965	0.014208	-0.858747
H	0.218933	3.452446	1.631250	H	-5.051403	1.539871	-0.496094
C	-0.321654	1.840633	3.586178	H	-2.807873	0.645220	-0.008153
H	0.743272	1.862987	3.339687	H	-2.241003	-3.143871	0.340945
H	-0.525621	2.604680	4.359463	C	2.458093	1.490249	1.368406
H	-0.559770	0.862586	4.013051	C	3.261224	0.998523	2.347951
C	-2.550058	1.891511	2.733615	H	3.995698	1.594358	2.871968
H	-3.184358	1.993747	1.852665	H	3.134429	-0.033371	2.648205
H	-2.699309	0.884436	3.132241	O	2.529945	2.824544	0.951720
H	-2.877353	2.625326	3.493985	C	3.474911	3.675017	1.578619

Atom	X	Y	Z	Atom	X	Y	Z
H	3.361907	4.657948	1.113791	N	3.051334	0.729920	-2.531269
H	3.289437	3.759116	2.657479	C	2.219292	1.263159	-3.616140
H	4.501800	3.316472	1.426928	H	2.822425	1.594816	-4.480714
N	3.297446	-1.797133	-0.987245	H	1.508887	0.501281	-3.948813
C	3.825155	-2.174523	0.333847	H	1.648016	2.117692	-3.246108
H	4.240108	-1.291674	0.827377	C	3.908819	1.794223	-1.990846
H	4.608731	-2.950000	0.257926	H	4.578828	2.213594	-2.763518
H	3.013168	-2.560171	0.953843	H	3.282944	2.590333	-1.582556
C	2.638753	-2.954627	-1.606756	H	4.519826	1.412496	-1.169447
H	2.168256	-2.672712	-2.552929	H	4.686279	-0.100435	-3.634632
H	3.350945	-3.777518	-1.800515	C	-1.266750	-2.288695	-1.651877
H	1.859491	-3.321248	-0.934401	H	-2.008943	-2.797089	-2.257312
C	4.373930	-1.268977	-1.842807	H	-0.449235	-2.912430	-1.311381
H	5.028874	-0.659074	-1.212942	H	-3.503974	-1.111132	-2.929330
H	4.999880	-2.084120	-2.250207	H	-3.057237	0.038485	-4.217256
C	3.840152	-0.422416	-2.999517	H	-2.315677	-1.585265	-4.183862
H	3.189088	-1.034167	-3.633385				

**Table 1 (continued)**



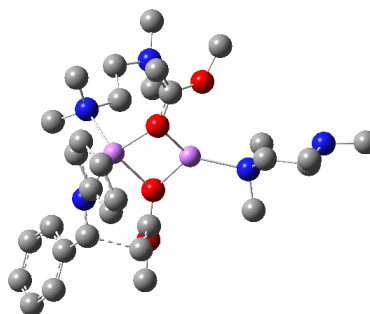
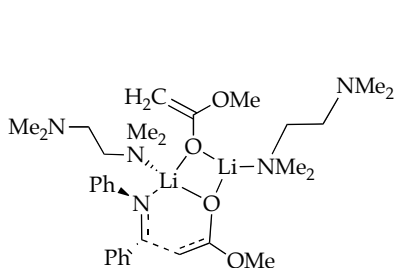
**5e**  
 $G = -1796.271617$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.054394	2.864835	-3.675036	H	3.916193	0.629920	2.760115
O	-0.133009	1.663046	-2.908641	N	-0.305213	2.068371	1.244723
C	-0.893578	1.626279	-1.772921	C	-1.417248	1.951633	2.088300
O	-0.888392	0.512773	-1.188878	C	-1.387903	0.929027	3.066421
Li	-1.685410	-1.149413	-0.805039	C	-2.444698	0.717338	3.944360
O	-0.573956	-1.618811	0.615148	C	-3.587885	1.522233	3.889486
Li	0.232053	0.079492	0.773301	C	-3.640985	2.540046	2.937248
N	2.304694	-0.357519	1.731752	C	-2.584433	2.755295	2.050225
C	3.015297	-1.077765	0.651518	H	-2.675785	3.563712	1.333369
C	4.448190	-1.556159	0.962688	H	-4.517695	3.181757	2.877967
N	4.932963	-2.528671	-0.019911	H	-4.413947	1.361412	4.576533
C	5.103535	-1.953038	-1.348305	H	-2.372093	-0.078824	4.681530
H	5.828406	-1.113103	-1.368129	H	-0.504220	0.301542	3.132750
H	5.466434	-2.725956	-2.034466	C	-0.254657	3.132787	0.429122
H	4.148132	-1.589525	-1.736514	C	1.026908	3.528155	-0.226961
C	6.168815	-3.154560	0.430870	C	1.972358	2.605074	-0.698261
H	6.006763	-3.641112	1.398992	C	3.145619	3.034023	-1.318681
H	6.476686	-3.922316	-0.287948	C	3.403479	4.397638	-1.478735
H	7.008363	-2.439125	0.544442	C	2.472383	5.328629	-1.015080
H	5.136541	-0.690504	1.044831	C	1.297778	4.895261	-0.399612
H	4.456136	-2.057435	1.937063	H	0.577928	5.627218	-0.039086
H	2.407345	-1.946118	0.379892	H	2.661346	6.393207	-1.127771
H	3.033156	-0.405616	-0.215309	H	4.319895	4.729849	-1.959187
C	2.019021	-1.215474	2.890460	H	3.859992	2.299153	-1.681543
H	1.449727	-2.094784	2.583324	H	1.780411	1.543500	-0.595808
H	2.930265	-1.542999	3.419441	H	-0.838896	4.016803	0.701457
H	1.414252	-0.651938	3.608488	C	-0.407658	-2.848280	1.007665
C	3.006774	0.854399	2.177553	C	-1.054536	-3.475394	2.024669
H	3.287928	1.463746	1.316189	H	-0.872502	-4.504121	2.303813
H	2.332547	1.448622	2.801357	H	-1.764608	-2.907333	2.612312



Atom	X	Y	Z	Atom	X	Y	Z
O	0.558451	-3.490265	0.229619	H	-3.554655	-1.158869	-3.278570
C	0.920411	-4.819023	0.567442	N	-2.016752	-2.365487	-2.557494
H	1.731432	-5.097307	-0.109820	C	-1.194094	-1.889214	-3.676761
H	1.273492	-4.887158	1.604500	H	-1.426946	-2.416781	-4.619362
H	0.078578	-5.512873	0.437505	H	-1.340667	-0.815538	-3.818698
N	-3.858881	-1.191192	-0.545372	H	-0.139128	-2.051636	-3.439270
C	-4.231567	-1.587489	0.821063	C	-1.714687	-3.776383	-2.279736
H	-3.740873	-2.531035	1.074912	H	-1.935252	-4.422661	-3.148728
H	-5.324273	-1.702603	0.936668	H	-0.659000	-3.868489	-2.016029
H	-3.884916	-0.826438	1.525161	H	-2.294275	-4.131416	-1.424098
C	-4.414204	0.132625	-0.852608	H	-3.849258	-2.880537	-3.539141
H	-4.084709	0.469613	-1.839549	C	-1.494282	2.785455	-1.229340
H	-5.519395	0.129594	-0.834824	H	-1.528486	3.701199	-1.809807
H	-4.056202	0.852619	-0.112187	H	-2.373734	2.593936	-0.626265
C	-4.283637	-2.201044	-1.530674	H	0.442715	3.663163	-3.115751
H	-4.175526	-3.186001	-1.066246	H	0.541650	2.614569	-4.554849
H	-5.352945	-2.091369	-1.787524	H	-1.049366	3.199131	-3.992473
C	-3.450011	-2.146147	-2.815099				

**Table 1 (continued)**

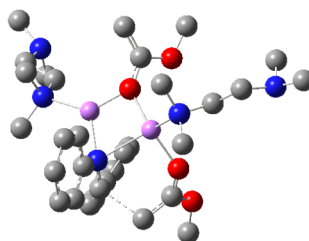
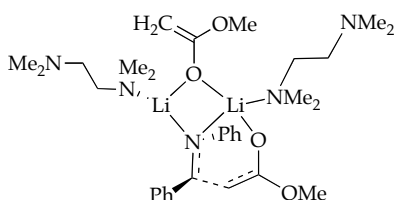


**5f**  
 $G = -1796.248546$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.499206	-1.151011	-3.863819	N	-2.244553	-1.481326	1.110921
O	-1.769102	-0.354649	-2.925329	C	-1.534260	-2.227359	2.059971
C	-1.211325	-0.924199	-1.829776	C	-1.355587	-1.646188	3.337252
O	-0.562873	-0.118232	-1.106597	C	-0.675471	-2.306356	4.353912
Li	1.217900	0.075443	-0.561841	C	-0.136776	-3.579299	4.139750
O	0.928032	0.232871	1.229038	C	-0.297444	-4.171363	2.887368
Li	-0.970662	0.194394	0.953656	C	-0.981099	-3.515410	1.862693
N	-1.565580	2.332674	1.413374	H	-1.079900	-4.015483	0.904363
C	-0.674662	3.076480	0.495184	H	0.115647	-5.160234	2.698391
C	-0.623206	4.608871	0.652821	H	0.395850	-4.096415	4.932943
N	0.280613	5.212782	-0.332061	H	-0.572167	-1.827969	5.325258
C	-0.317064	5.296278	-1.659904	H	-1.793244	-0.667071	3.517599
H	-1.210638	5.952494	-1.689841	C	-2.763096	-2.149938	0.056618
H	0.418411	5.695057	-2.367157	C	-3.989563	-1.604504	-0.610555
H	-0.613634	4.304999	-2.013452	C	-4.320790	-0.244830	-0.576343
C	0.747510	6.524645	0.098621	C	-5.475967	0.224902	-1.201374
H	1.257548	6.439572	1.063914	C	-6.330391	-0.659071	-1.864155
H	1.465319	6.916132	-0.631064	C	-6.019938	-2.020696	-1.892431
H	-0.067511	7.268677	0.203995	C	-4.859897	-2.485469	-1.271895
H	-1.635551	5.054020	0.593138	H	-4.627945	-3.548867	-1.290008
H	-0.232710	4.848636	1.647593	H	-6.685535	-2.722423	-2.389068
H	0.338219	2.688336	0.632040	H	-7.234312	-0.292963	-2.343871
H	-0.985518	2.811369	-0.521498	H	-5.715242	1.285003	-1.163364
C	-1.186188	2.479346	2.827537	H	-3.670707	0.433416	-0.039534
H	-0.136310	2.206284	2.965690	H	-2.838365	-3.239909	0.150974
H	-1.349567	3.501016	3.210684	C	1.887288	0.717877	1.963698
H	-1.798783	1.799954	3.430625	C	2.058656	0.594843	3.299899
C	-2.979455	2.680806	1.232347	H	2.895588	1.023706	3.833253
H	-3.239188	2.629340	0.170308	H	1.357370	-0.016287	3.853094
H	-3.602065	1.964616	1.778484	O	2.783647	1.433211	1.149267
H	-3.225869	3.691601	1.597728	C	3.901548	2.051703	1.767204

Atom	X	Y	Z	Atom	X	Y	Z
H	4.456356	2.558457	0.973281	H	4.550882	1.312033	2.252819
C	7.410952	-1.878612	-1.617080	N	6.124889	-1.784244	-0.937861
H	7.650865	-0.921582	-2.093301	H	3.007945	-1.184851	-3.867255
H	7.439544	-2.666470	-2.396260	H	1.913111	-2.032902	-2.744945
H	8.195947	-2.099898	-0.885928	H	1.394421	-0.521371	-3.516501
C	5.828142	-3.019567	-0.219685	C	3.193867	1.060734	-2.340607
H	4.925158	-2.907755	0.386594	H	4.007686	1.041886	-3.082840
H	5.689299	-3.888824	-0.894032	H	2.347390	1.594514	-2.786701
H	6.654448	-3.248721	0.461008	H	3.525620	1.615520	-1.459227
C	5.064672	-1.401650	-1.869704	H	3.270532	-1.911232	-0.747007
H	5.430403	-0.536049	-2.433951	C	-1.455743	-2.273924	-1.447609
H	4.865520	-2.203531	-2.609951	H	-1.890892	-2.948256	-2.178976
C	3.766120	-1.014258	-1.136602	H	-0.647933	-2.711580	-0.869049
H	4.020786	-0.386612	-0.277186	H	-3.407504	-1.559814	-3.414670
N	2.750667	-0.280830	-1.929421	H	-2.766000	-0.471495	-4.674952
C	2.250023	-1.046562	-3.080043	H	-1.876691	-1.962794	-4.257699
H	3.582423	2.788880	2.514619				

**Table 1 (continued)**

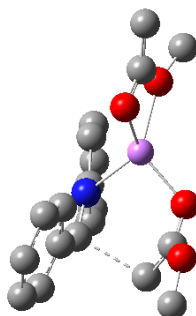
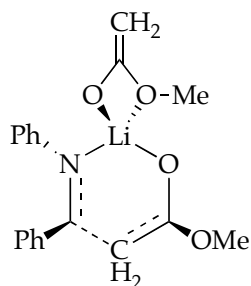


**5g**  
 $G = -1796.26004$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	0.626985	2.291510	4.573910	C	0.507172	1.953803	-2.662571
O	1.215148	1.441800	3.589318	C	0.975274	2.640317	-3.778692
C	1.381756	1.875177	2.312535	C	1.106086	4.032621	-3.756181
O	1.948851	1.070845	1.552454	C	0.762192	4.714752	-2.589089
Li	1.486749	0.290377	-0.111422	C	0.290290	4.036248	-1.464516
O	0.317033	-1.056085	-0.796724	H	0.041767	4.614106	-0.581400
Li	-1.098278	0.054884	-0.978676	H	0.864339	5.796962	-2.545317
N	-3.070775	-0.124519	-1.640711	H	1.472834	4.570148	-4.625798
C	-3.623049	-1.252694	-0.852950	H	1.242860	2.081666	-4.672871
C	-5.037657	-1.738168	-1.224310	H	0.439290	0.867755	-2.691389
N	-5.480978	-2.798643	-0.317138	C	-0.792412	2.487665	0.704773
C	-5.944514	-2.280981	0.965133	C	-1.632831	1.715468	1.668802
H	-6.849357	-1.646990	0.870332	C	-1.449545	0.342740	1.911029
H	-6.185372	-3.117299	1.630224	C	-2.265356	-0.333336	2.821459
H	-5.164997	-1.686565	1.449563	C	-3.280040	0.341640	3.503861
C	-6.498722	-3.646833	-0.924874	C	-3.473314	1.705909	3.270610
H	-6.112202	-4.088183	-1.849544	C	-2.656519	2.382404	2.364607
H	-6.749895	-4.463879	-0.239479	H	-2.813456	3.444514	2.186885
H	-7.436326	-3.106765	-1.165498	H	-4.261882	2.243007	3.791668
H	-5.755433	-0.894871	-1.244260	H	-3.910220	-0.187424	4.213839
H	-5.015332	-2.156093	-2.236483	H	-2.095701	-1.391552	3.001680
H	-2.933305	-2.098358	-0.957465	H	-0.657024	-0.202444	1.406590
H	-3.595458	-0.942903	0.196217	H	-1.161455	3.511089	0.590488
C	-2.962175	-0.434174	-3.076405	C	0.379986	-2.354742	-0.929883
H	-2.428168	-1.380903	-3.204222	C	0.110230	-3.057429	-2.060862
H	-3.941394	-0.508807	-3.575683	H	0.170194	-4.134910	-2.123113
H	-2.392594	0.358836	-3.573523	H	-0.135059	-2.512422	-2.964695
C	-3.792052	1.140555	-1.432829	O	0.769521	-2.950024	0.258054
H	-3.858074	1.351730	-0.361982	C	0.876839	-4.363620	0.290200
H	-3.233238	1.952803	-1.908569	H	1.190984	-4.623795	1.303735
H	-4.808578	1.127515	-1.856204	H	-0.086762	-4.842331	0.071904
N	-0.346963	1.848907	-0.413711	H	1.623065	-4.726195	-0.429108
C	0.135665	2.627847	-1.469876	C	0.825593	3.119813	1.858996

Atom	X	Y	Z	Atom	X	Y	Z
H	0.441474	3.825847	2.588828	H	7.674873	-3.073108	1.726857
H	1.388887	3.577651	1.052073	H	7.557370	-3.224624	-0.044706
H	-0.420677	2.507502	4.341564	H	5.394298	-2.199558	-1.121041
H	0.681301	1.734052	5.510780	H	6.058419	-0.737961	-0.377144
H	1.185810	3.228831	4.677121	H	3.931526	-0.545944	1.022809
N	3.449380	-0.039401	-0.945381	H	3.225181	-1.841445	0.060743
C	3.953706	-1.024203	0.038431	C	4.187156	1.229338	-0.924930
C	5.372089	-1.575177	-0.204892	H	4.202337	1.619052	0.096607
N	5.881063	-2.314245	0.952645	H	5.224016	1.138941	-1.290447
C	5.149709	-3.551340	1.198865	H	3.668269	1.952029	-1.563573
H	5.202085	-4.261773	0.348188	C	3.364765	-0.583633	-2.307014
H	5.568170	-4.049268	2.080285	H	2.777736	-1.506803	-2.298901
H	4.096751	-3.342147	1.404877	H	2.854983	0.142432	-2.947891
C	7.307273	-2.578012	0.820974	H	4.353089	-0.791038	-2.749913
H	7.850669	-1.633659	0.706035				

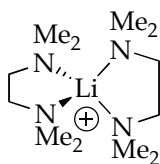
**Table 1 (continued)**



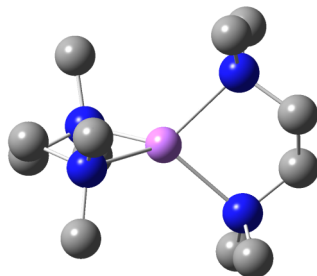
**5h (part 1)**  
**7b (part 1)**  
*G* = -1096.125087  
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	3.810699	2.395381	0.723651	C	-2.013357	0.775909	-1.233472
O	2.483869	2.144718	0.323709	H	-1.091884	1.344062	-1.146228
C	1.695557	3.192373	-0.284702	H	-3.128299	2.481143	-1.902509
O	0.500798	2.775007	-0.419258	H	-5.261761	1.223242	-2.188303
Li	0.698764	1.081083	0.440973	H	-5.319626	-1.218879	-1.681644
O	-0.023742	0.380764	2.081382	H	-3.276053	-2.360120	-0.872824
C	-1.103583	-0.245211	2.090215	C	1.496461	-1.604956	-0.521685
C	-1.241959	-1.598676	1.702222	C	2.738452	-1.017697	-0.865591
H	-2.187097	-2.119778	1.814005	C	3.920169	-1.748812	-0.842080
H	-0.353886	-2.203195	1.845220	C	3.921026	-3.098758	-0.470988
O	-2.208492	0.529019	2.386500	C	2.709826	-3.693552	-0.116021
C	-3.482565	-0.080557	2.508750	C	1.518205	-2.968332	-0.136406
H	-4.163467	0.708518	2.840766	H	0.601188	-3.467482	0.158630
H	-3.839436	-0.480077	1.552706	H	2.687628	-4.739130	0.188324
H	-3.474796	-0.886354	3.256407	H	4.846396	-3.669869	-0.451972
N	0.367419	-0.790923	-0.599560	H	4.852918	-1.260585	-1.118833
C	-0.835203	-1.341771	-0.477847	H	2.742436	0.031539	-1.144951
H	-0.953647	-2.423977	-0.594089	C	2.282618	4.378442	-0.602826
C	-2.041741	-0.594119	-0.923914	H	3.330177	4.589913	-0.433980
C	-3.248144	-1.295044	-1.098308	H	1.670658	5.150443	-1.053610
C	-4.399408	-0.652834	-1.549653	H	3.862573	3.229487	1.437418
C	-4.366296	0.714944	-1.836827	H	4.177831	1.481211	1.200169
C	-3.171063	1.418514	-1.676574	H	4.452301	2.635577	-0.137020

**Table 1 (continued)**



**S10**



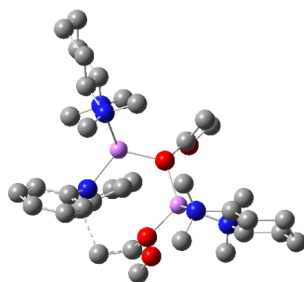
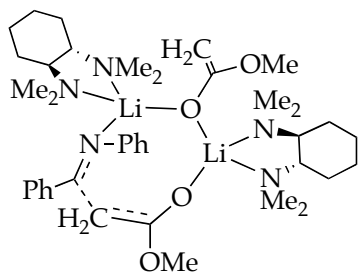
**5h (part 2)**

$G = -700.0090158$

(-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000036	-0.000067	0.000879	N	-1.582491	1.067730	-1.066734
N	1.582060	-1.073170	-1.061697	C	-2.758167	0.226867	-0.731418
C	2.757437	-0.229782	-0.731708	C	-2.760985	-0.230160	0.726264
C	2.761419	0.234317	0.723736	N	-1.583853	-1.066708	1.067337
N	1.584244	1.072099	1.061734	C	-1.447203	-1.151090	2.535448
C	1.447954	1.162431	2.529548	H	-0.576993	-1.763608	2.790272
H	2.336140	1.617627	2.996896	H	-1.306447	-0.151750	2.956048
H	0.577837	1.776033	2.782081	H	-2.335259	-1.604413	3.004863
H	1.307219	0.164807	2.954208	C	-1.749742	-2.434049	0.531841
C	1.749888	2.437257	0.520654	H	-0.893866	-3.046969	0.824923
H	1.804648	2.420497	-0.571128	H	-2.664699	-2.911287	0.919007
H	0.893850	3.051189	0.811129	H	-1.804431	-2.421852	-0.560012
H	2.664711	2.916255	0.905935	H	-2.756694	0.639919	1.390777
H	2.758126	-0.632537	1.392443	H	-3.698687	-0.774009	0.930332
H	3.699087	0.779508	0.924297	H	-3.696880	0.767202	-0.940262
H	3.696350	-0.770396	-0.938943	H	-2.747164	-0.643266	-1.395845
H	2.745043	0.637153	-1.400280	C	-1.753450	2.433035	-0.527644
C	1.441073	-1.170094	-2.528648	H	-0.899552	3.049646	-0.818718
H	1.297113	-0.174588	-2.957131	H	-2.669827	2.908166	-0.914055
H	2.328628	-1.625568	-2.996929	H	-1.808563	2.417850	0.564130
H	0.571322	-1.786465	-2.775667	C	-1.442536	1.156981	-2.534246
C	1.754332	-2.435543	-0.515680	H	-0.572658	1.771619	-2.785111
H	2.670990	-2.911869	-0.899927	H	-1.299392	0.159200	-2.957685
H	1.809673	-2.414693	0.575979	H	-2.330203	1.610454	-3.004256
H	0.900855	-3.054322	-0.803374				

**Table 1 (continued)**



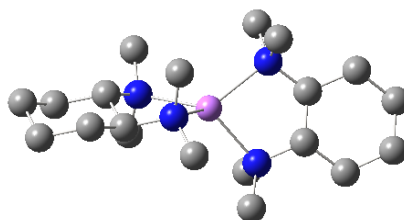
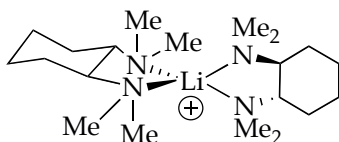
**7a**  
 $G = -2107.099098$   
 (-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.882295	4.843801	0.414028	C	-0.584057	-0.860684	-2.148942
O	-2.056096	3.428864	0.422712	C	-0.765717	-2.113434	-2.649616
C	-1.438922	2.662951	1.382733	C	-0.427180	3.206533	2.216231
O	-1.750479	1.451784	1.360701	H	-0.338896	4.284110	2.310496
Li	-2.036523	0.082043	0.090695	H	-0.279534	2.662512	3.143242
O	-0.433486	-0.516495	-0.900382	H	-0.851684	5.123042	0.176391
Li	1.354391	-0.250125	-0.091692	H	-2.546103	5.219395	-0.368058
N	1.447563	1.250964	1.370478	H	-2.171689	5.284048	1.376079
C	1.746797	0.737413	2.652802	N	-4.087319	0.291679	-0.865799
C	0.783169	-0.002006	3.365347	C	-4.998878	-0.688599	-0.213450
C	1.072291	-0.539578	4.620364	C	-3.833408	0.029031	-2.290244
C	2.330177	-0.354910	5.199296	C	-4.571780	1.668325	-0.698755
C	3.293672	0.387146	4.510882	C	-4.234594	-1.940016	0.286533
C	3.005243	0.930898	3.258130	C	-6.216728	-1.093393	-1.076808
H	3.758838	1.505578	2.724324	H	-5.393035	-0.174404	0.672061
H	4.276477	0.542527	4.950864	H	-4.718457	0.200115	-2.925476
H	2.555194	-0.777280	6.175076	H	-3.036199	0.696878	-2.626348
H	0.307393	-1.100535	5.153487	H	-3.481029	-0.995373	-2.436021
H	-0.199634	-0.113205	2.917670	H	-3.833849	2.360294	-1.108943
C	1.350234	2.591480	1.348519	H	-5.540244	1.843206	-1.201039
C	1.348144	3.327332	0.048724	H	-4.673656	1.898644	0.364624
C	0.720663	2.823502	-1.101288	C	-5.202461	-2.935425	0.971197
C	0.731929	3.555029	-2.290167	H	-3.804861	-2.437364	-0.594029
C	1.371528	4.795415	-2.358146	N	-3.065830	-1.561557	1.127738
C	2.004480	5.302907	-1.221194	C	-7.158655	-2.062701	-0.352246
C	1.989579	4.574398	-0.030824	H	-5.867587	-1.578032	-1.997603
H	2.483142	4.975174	0.852574	H	-6.760213	-0.191495	-1.384578
H	2.512634	6.263416	-1.260644	C	-6.394435	-3.316602	0.084175
H	1.377736	5.360816	-3.286692	H	-4.653075	-3.835883	1.270568
H	0.231336	3.145689	-3.163675	H	-5.590127	-2.485177	1.894863
H	0.210874	1.866299	-1.069044	C	-2.106432	-2.661682	1.263103
H	1.885367	3.145177	2.129898	C	-3.410347	-1.037501	2.457928



Atom	X	Y	Z	Atom	X	Y	Z
H	-7.593647	-1.572977	0.531491	C	5.931853	-3.595041	-0.784800
H	-7.997904	-2.327933	-1.007569	H	-1.207713	-2.288501	1.764097
H	-6.039081	-3.855105	-0.806643	H	-2.494106	-3.510177	1.853172
H	-7.055109	-4.006870	0.623783	H	-1.819783	-3.020785	0.271601
H	-0.899494	-2.320217	-3.702449	H	-4.142498	-0.231658	2.375314
H	-0.791185	-2.953943	-1.968962	H	-3.807292	-1.810601	3.136243
O	-0.556893	0.261103	-2.981420	H	-2.513100	-0.606645	2.907935
C	-0.684396	0.069382	-4.379353	N	2.463792	-2.297120	0.455394
H	-0.617001	1.060780	-4.834741	H	3.907966	-4.303368	-0.880202
H	0.118253	-0.566740	-4.775612	H	4.510725	-4.130855	0.762573
H	-1.650221	-0.383548	-4.640257	C	5.932382	-2.927013	-2.162419
C	3.831937	-2.263378	-0.129498	H	5.300524	-1.054863	-3.060008
C	1.560320	-3.251711	-0.201831	H	5.936553	-0.911205	-1.427183
C	2.508127	-2.586834	1.894533	C	2.794963	0.203550	-2.816654
C	3.860130	-1.557536	-1.507069	C	4.032866	0.827820	-0.852340
C	4.505750	-3.656021	-0.225204	H	6.577625	-3.023883	-0.101574
H	4.426591	-1.657250	0.567141	H	6.354055	-4.606408	-0.841502
H	1.840829	-4.303971	-0.026750	H	5.366243	-3.549301	-2.871086
H	0.553417	-3.099392	0.191790	H	6.952934	-2.851046	-2.558698
H	1.514122	-3.067967	-1.276703	H	2.239601	1.140511	-2.744164
H	1.503280	-2.491525	2.311449	H	3.650784	0.363598	-3.495303
H	2.871401	-3.604944	2.117729	H	2.135548	-0.552500	-3.251187
H	3.146521	-1.862529	2.405693	H	3.427596	1.726920	-0.727334
C	5.302274	-1.532115	-2.073053	H	4.366624	0.513130	0.139754
H	3.251034	-2.157424	-2.195624	H	4.916229	1.087223	-1.458366
N	3.203684	-0.220880	-1.469462				

Table 1 (cont..)

**7b (part 2)** $G = -1010.821826$ 

(-60 °C)

Atom	X	Y	Z	Atom	X	Y	Z
C	5.507338	0.357428	0.162202	Li	0.000008	0.179886	0.024431
C	4.279239	0.909065	0.896067	C	-2.765206	-0.746662	0.326312
C	2.965687	0.688421	0.110469	C	-2.976633	0.691398	-0.203238
C	2.777506	-0.804014	-0.253213	C	-4.239129	0.779580	-1.091216
C	4.046762	-1.369223	-0.935470	C	-5.495038	0.264232	-0.377987
C	5.322502	-1.135897	-0.116599	C	-5.283836	-1.183015	0.072464
H	5.267274	-1.684865	0.834359	C	-4.057013	-1.284065	0.988452
H	6.183548	-1.540472	-0.660303	H	-3.907555	-2.324283	1.296441
H	3.915683	-2.439734	-1.127606	H	-4.266640	-0.712647	1.901509
H	4.180942	-0.888492	-1.912580	H	-5.148687	-1.826866	-0.808446
H	2.627942	-1.359364	0.683632	H	-6.166269	-1.559707	0.601620
N	1.514464	-1.025008	-1.039580	H	-5.720968	0.894827	0.493669
C	1.162139	-2.458181	-1.078867	H	-6.356261	0.340854	-1.051078
H	0.162494	-2.573941	-1.510675	H	-4.095997	0.180917	-1.999182
H	1.857244	-3.053645	-1.687875	H	-4.385021	1.816341	-1.416630
H	1.153194	-2.868739	-0.066483	H	-3.154734	1.335916	0.665626
C	1.602207	-0.537250	-2.431723	N	-1.732266	1.235177	-0.852909
H	1.842325	0.529097	-2.457142	C	-1.629102	0.894287	-2.286688
H	2.351298	-1.075956	-3.027371	H	-0.654248	1.221285	-2.657730
H	0.634357	-0.681293	-2.917236	H	-1.708773	-0.187486	-2.430373
H	3.053672	1.246880	-0.829775	H	-2.397879	1.381604	-2.901548
N	1.748024	1.255297	0.789427	C	-1.684386	2.704664	-0.718206
C	1.716996	0.991970	2.242866	H	-2.534487	3.203628	-1.207707
H	0.763657	1.344655	2.644127	H	-1.683491	2.984709	0.339431
H	1.799418	-0.081138	2.440809	H	-0.766574	3.083640	-1.176311
H	2.516807	1.507536	2.791158	H	-2.540583	-1.391963	-0.535829
C	1.672178	2.714265	0.576362	N	-1.545997	-0.837088	1.201197
H	2.528503	3.253318	1.008213	C	-1.216330	-2.244059	1.504503
H	1.632098	2.933871	-0.494634	H	-1.929292	-2.711846	2.198178
H	0.763515	3.104220	1.043714	H	-1.199822	-2.830269	0.582642
H	4.215422	0.406850	1.869305	H	-0.224919	-2.291722	1.967137
H	4.408430	1.978051	1.101358	C	-1.682965	-0.110881	2.480890

Atom	X	Y	Z	Atom	X	Y	Z
H	5.657342	0.896062	-0.784285	H	-1.840758	0.957370	2.310147
H	6.404152	0.532553	0.766930	H	-2.504209	-0.488384	3.105011
				H	-0.759247	-0.232066	3.051263

#### Part 4. Full References

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