Computational Studies of Lithium Diisopropylamide Deaggregation

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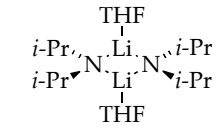
Supporting Information

Scheme 1



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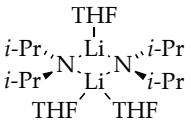

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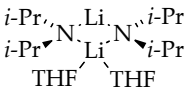

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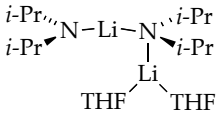

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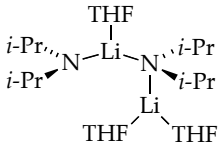

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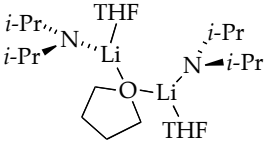

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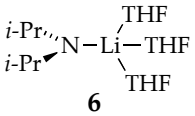

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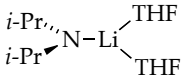

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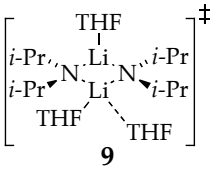

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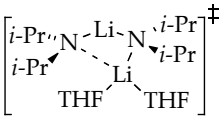

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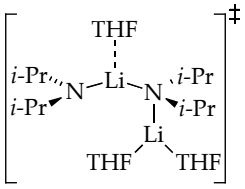

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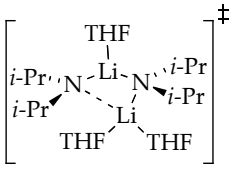

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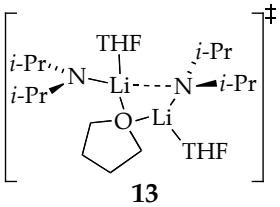

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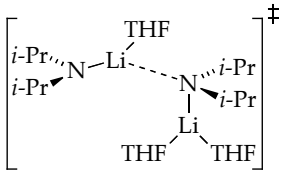

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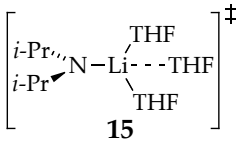

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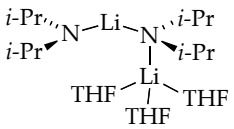

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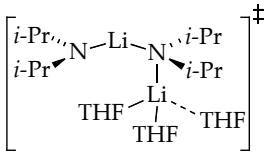

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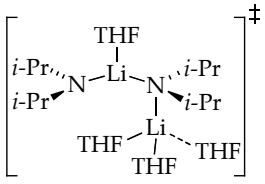

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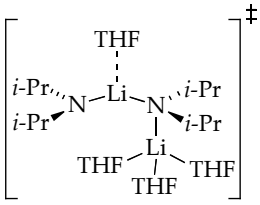

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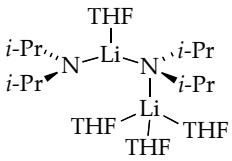

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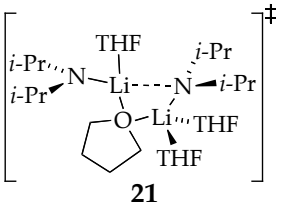

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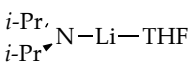

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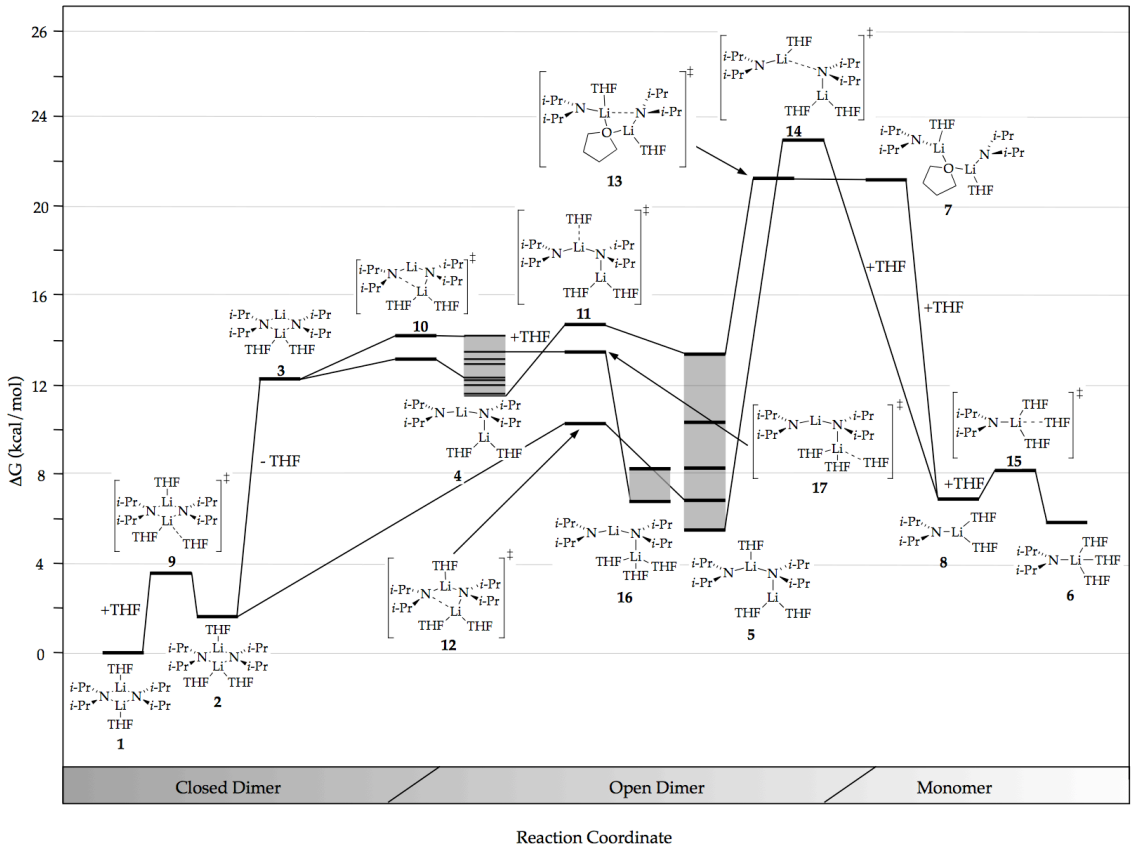
Scheme 2 (*Scheme 2* in paper)



Scheme 3 (*Scheme 6* in paper)

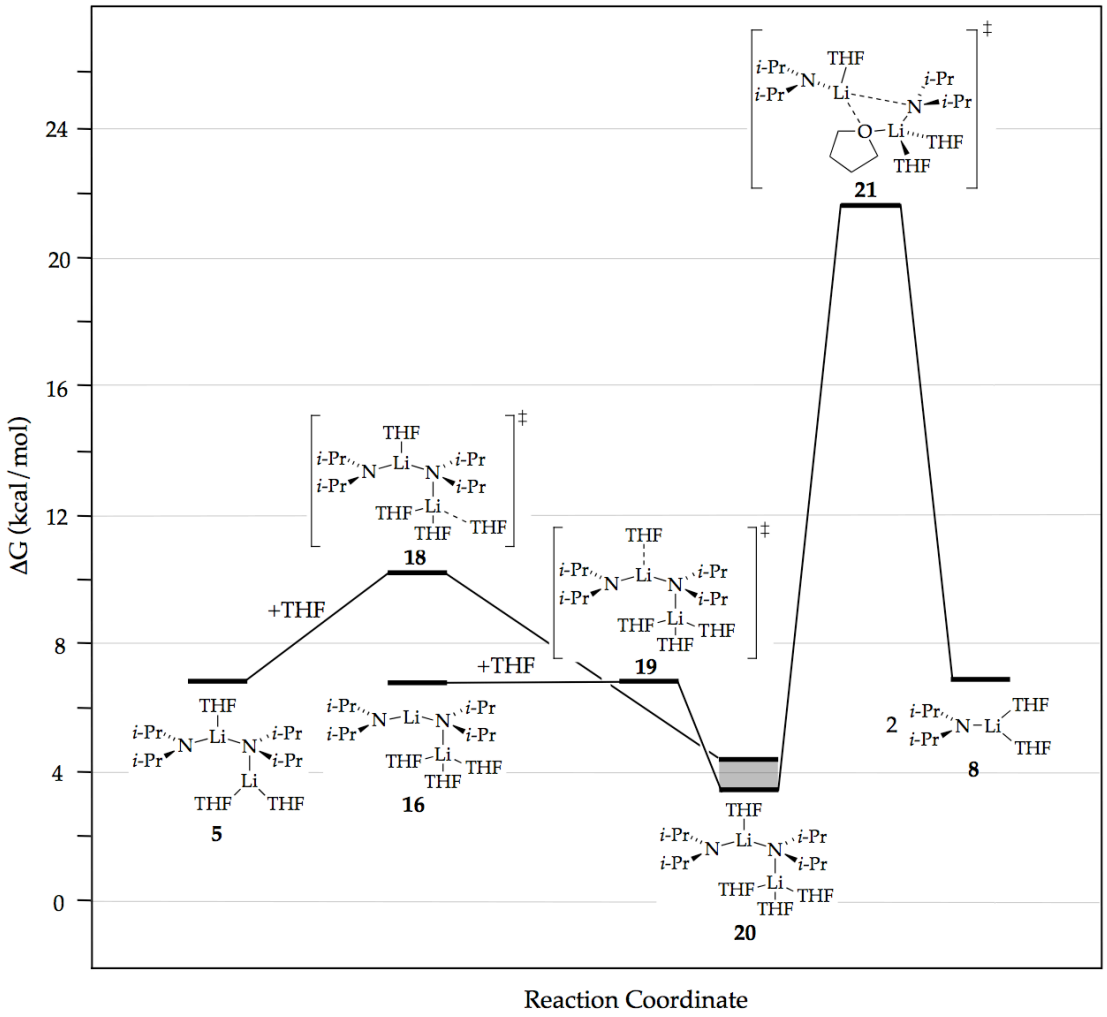
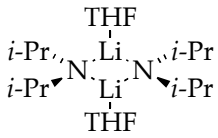
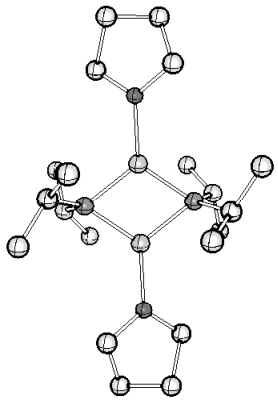


Table 1. Optimized geometries at the B3LYP level of theory with 6-31G(d) basis set of THF disolvated, trisolvated and tetrasolvated LDA aggregates including closed and open dimers as well as monomers at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z). Single point MP2 energies are included. $\Delta G^{\ddagger}$ and ΔG (when reported) is the difference in free energy relative to disolvated LDA dimer **1**.



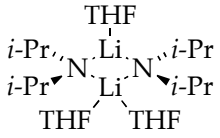


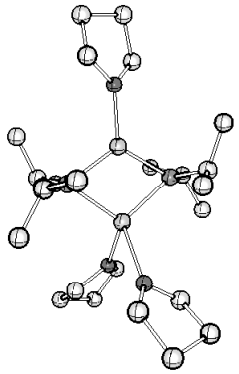
1
G = -1063.135499
G_{MP2} = -1059.343827

Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.194627	-0.007825	0.022332	C	4.032339	-1.143606	0.199177
N	0.013907	1.643769	0.077205	C	5.437966	-0.758062	-0.271094
C	0.196558	2.410032	1.319032	C	5.411742	0.774063	-0.154916
C	1.159764	1.707079	2.290512	C	3.984087	1.095274	-0.593500
H	2.159075	1.604292	1.849772	H	3.902781	1.157446	-1.686665
H	1.262404	2.264200	3.230548	H	3.572808	2.009642	-0.160821
H	0.802179	0.701928	2.550069	H	6.162143	1.270000	-0.777688
C	-1.131524	2.719155	2.048700	H	5.571005	1.083108	0.884979
H	-1.598978	1.790545	2.404654	H	5.590704	-1.057380	-1.314703
H	-0.983501	3.376104	2.917980	H	6.219980	-1.226951	0.333343
H	-1.838550	3.216969	1.374689	H	3.991648	-1.300598	1.282899
H	0.658344	3.392275	1.104388	H	3.630188	-2.031035	-0.296809
Li	1.194600	0.007938	0.022158	C	-0.277970	2.554246	-1.035528
N	-0.013962	-1.643687	0.077247	C	-0.932408	1.814820	-2.212599
C	-0.196637	-2.409858	1.319127	H	-1.876483	1.339255	-1.919253
C	1.131405	-2.718766	2.048953	H	-1.147122	2.498323	-3.043671
H	1.598735	-1.790078	2.404863	H	-0.264714	1.033138	-2.596792
H	0.983363	-3.375653	2.918275	C	0.961585	3.312183	-1.569417
H	1.838548	-3.216575	1.375059	H	1.655983	2.609117	-2.049010
C	-1.160039	-1.706940	2.290445	H	0.685387	4.074299	-2.312169
H	-2.159328	-1.604365	1.849606	H	1.500736	3.820562	-0.761989
H	-1.262680	-2.263956	3.230543	H	-1.002510	3.335320	-0.721398
H	-0.802631	-0.701703	2.549918	O	-3.182976	0.015599	-0.128112
H	-0.658276	-3.392178	1.104519	C	-3.983928	-1.095127	-0.594129
C	0.278101	-2.554233	-1.035377	C	-5.411404	-0.774615	-0.154519
C	-0.961328	-3.312344	-1.569312	C	-5.438354	0.757507	-0.270589
H	-1.655760	-2.609392	-2.049018	C	-4.032490	1.143719	0.198539
H	-0.684990	-4.074495	-2.311978	H	-3.991063	1.301394	1.282122

Table 1 (continued).

H	-1.500486	-3.820717	-0.761885	H	-3.630993	2.030985	-0.298285
C	0.932582	-1.814844	-2.212451	H	-6.220074	1.226032	0.334511
H	1.876607	-1.339195	-1.919069	H	-5.592104	1.056795	-1.314054
H	1.147416	-2.498388	-3.043457	H	-5.569779	-1.083823	0.885463
H	0.264859	-1.033240	-2.596749	H	-6.162035	-1.270817	-0.776806
H	1.002689	-3.335209	-0.721109	H	-3.903299	-1.156675	-1.687391
O	3.182976	-0.015444	-0.127663	H	-3.572024	-2.009558	-0.162195



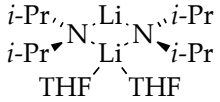


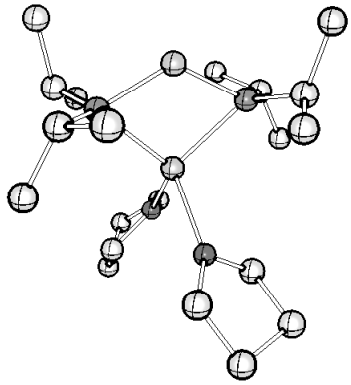
2
G = -1295.468552
G_{MP2} = -1290.911118
ΔG = 10.2 kcal/mol
ΔG_{MP2} = 1.6 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
Li	0.818515	-0.011749	0.004258	H	-6.633962	-0.029432	1.356314
N	-0.496059	-1.437484	0.988166	H	-6.620794	0.423336	-1.339571
C	-0.681340	-2.820306	0.515699	H	-5.838785	1.620894	-0.288742
C	-0.333526	-2.984896	-0.967682	H	-3.951622	1.036081	-1.700686
H	0.670807	-2.607385	-1.178994	H	-4.495241	-0.657976	-1.834598
H	-0.381100	-4.040340	-1.266183	C	-0.453127	-1.446768	2.457559
H	-1.040201	-2.437207	-1.601717	C	-0.775698	-0.071705	3.052081
C	-2.113477	-3.378256	0.727230	H	-1.767842	0.274567	2.733930
H	-2.829240	-2.817093	0.111600	H	-0.768881	-0.099513	4.149612
H	-2.178574	-4.438251	0.443040	H	-0.043473	0.678653	2.735678
H	-2.434446	-3.302876	1.772178	C	0.891450	-1.938843	3.048504
H	-0.007660	-3.513315	1.059369	H	1.700346	-1.247902	2.782079
Li	-1.642109	-0.068981	0.010468	H	0.851865	-2.012142	4.144778
N	-0.569511	1.360057	-0.965104	H	1.158485	-2.930282	2.665912
C	-0.549529	1.365185	-2.434744	H	-1.219905	-2.131912	2.868840
C	0.748338	1.941691	-3.054151	O	2.485894	1.082386	1.028619
H	1.608142	1.312977	-2.792467	C	3.164391	1.956383	0.097963
H	0.684827	1.994694	-4.150329	C	3.776576	3.069184	0.948373
H	0.952920	2.955213	-2.691895	C	4.115724	2.319506	2.245463
C	-0.786821	-0.033966	-3.012818	C	2.934390	1.352405	2.374768
H	-1.748285	-0.444678	-2.678085	H	2.105362	1.801073	2.936113
H	-0.797335	-0.016146	-4.110432	H	3.200641	0.404757	2.851643
H	-0.000717	-0.729344	-2.700209	H	4.214220	2.974542	3.116342
H	-1.367862	1.992878	-2.839386	H	5.055614	1.766125	2.130254

Table 1 (continued).

C	-0.791028	2.733856	-0.483994	H	3.035753	3.853730	1.140987
C	-2.229862	3.269764	-0.707945	H	4.647250	3.530557	0.472262
H	-2.944776	2.684342	-0.113865	H	3.937435	1.380593	-0.428505
H	-2.316965	4.321898	-0.401935	H	2.426359	2.301410	-0.629022
H	-2.536145	3.213526	-1.758343	O	2.525183	-1.005662	-1.041557
C	-0.470385	2.886557	1.006609	C	3.282317	-1.819904	-0.116349
H	0.538433	2.528638	1.229448	C	3.958762	-2.894665	-0.967381
H	-0.545946	3.936783	1.317484	C	4.206898	-2.142148	-2.283001
H	-1.175044	2.315104	1.621929	C	2.948149	-1.276745	-2.395801
H	-0.123400	3.447978	-1.007964	H	2.141299	-1.808150	-2.915950
O	-3.634504	-0.116304	-0.021547	H	3.119497	-0.324230	-2.904790
C	-4.443741	0.217064	-1.172605	H	4.337341	-2.801529	-3.146378
C	-5.818902	0.572918	-0.610332	H	5.100957	-1.512412	-2.199075
C	-5.914867	-0.365209	0.603246	H	3.277713	-3.737798	-1.130865
C	-4.476736	-0.361501	1.130763	H	4.873836	-3.279474	-0.506742
H	-4.170055	-1.307364	1.583443	H	4.020134	-1.183456	0.389667
H	-4.313695	0.447729	1.853649	H	2.585845	-2.211297	0.628166
H	-6.203684	-1.373366	0.283550				





3
G = -1063.113999
G_{MP2} = -1059.324336
ΔG = 13.5 kcal/mol
ΔG_{MP2} = 12.2 kcal/mol

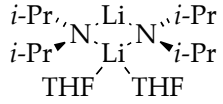
Closed dimer **3** connects directly to closed trisolvated LDA dimer **2**.

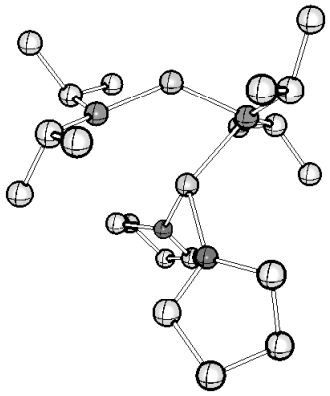
Atom	X	Y	Z	Atom	X	Y	Z
C	-1.953915	-0.136916	-2.517778	H	1.626270	-2.544548	-0.586163
N	-2.024230	0.029074	-1.058690	C	-0.811157	-4.348437	1.104056
Li	-1.904250	-1.470243	0.151949	H	-1.307975	-4.297854	2.079484
N	-0.336937	-1.879002	1.223499	H	-0.356528	-5.345170	1.011557
Li	0.023702	-0.044634	0.021905	H	-1.588008	-4.266697	0.327871
O	1.937212	0.002412	-0.935458	H	1.040154	-3.438806	1.661016
C	3.051478	0.059134	-0.011461	C	-0.332962	-1.675119	2.680124
C	4.311359	0.093857	-0.878408	C	-1.404666	-0.675490	3.126741
C	3.875639	-0.724117	-2.102568	H	-1.258839	0.300245	2.649954
C	2.415969	-0.296308	-2.267214	H	-1.382290	-0.520484	4.213066

Table 1 (continued).

H	2.327547	0.607633	-2.883771	H	-2.409658	-1.031852	2.862883
H	1.779764	-1.073852	-2.696120	C	1.043445	-1.230583	3.229173
H	4.472169	-0.522808	-2.997389	H	1.832068	-1.931995	2.933756
H	3.936390	-1.796686	-1.885488	H	1.048663	-1.170851	4.326877
H	4.550863	1.123294	-1.171472	H	1.311355	-0.243640	2.831314
H	5.181985	-0.323826	-0.363958	H	-0.572185	-2.622209	3.201357
H	3.019242	-0.832546	0.625842	C	-3.088752	0.997500	-0.744366
H	2.919149	0.943055	0.616290	C	-4.514070	0.402510	-0.866118
O	0.533347	1.911470	0.805633	H	-4.680047	-0.065430	-1.842203
C	0.624702	2.553275	2.098409	H	-5.290539	1.168621	-0.730117
C	1.041869	3.999220	1.820894	H	-4.666849	-0.368949	-0.096396
C	0.405735	4.255187	0.446469	C	-2.944352	1.598084	0.658044
C	0.599648	2.905915	-0.246046	H	-3.091831	0.834575	1.431541
H	-0.170929	2.664029	-0.981030	H	-3.696816	2.378452	0.829139
H	1.582995	2.837443	-0.729150	H	-1.950937	2.031508	0.803168
H	-0.661551	4.479883	0.554799	H	-3.052024	1.852986	-1.448053
H	0.873507	5.077643	-0.103036	C	-1.152640	0.980795	-3.227019
H	0.695842	4.687833	2.597396	H	-1.547843	1.970952	-2.971523
H	2.133776	4.079722	1.757312	H	-1.194285	0.884196	-4.321275
H	1.342965	1.999593	2.709298	H	-0.099009	0.951393	-2.922220
H	-0.356735	2.503763	2.585670	C	-1.380139	-1.501148	-2.913505
C	0.228801	-3.212084	0.943667	H	-0.361634	-1.624260	-2.529032
C	0.864046	-3.317289	-0.447193	H	-1.338342	-1.621800	-4.003570
H	0.113681	-3.198088	-1.236892	H	-1.993914	-2.317879	-2.509925
H	1.332200	-4.299540	-0.592136	H	-2.966705	-0.101901	-2.960703

Table 1 (continued).





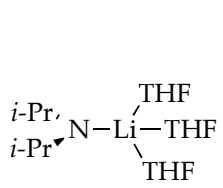
3*
G = -1063.113625
G_{MP2} = -1059.323335
ΔG = 13.7 kcal/mol
ΔG_{MP2} = 12.9 kcal/mol

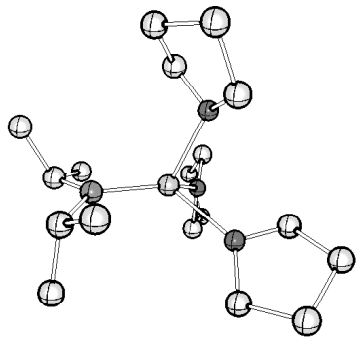
Closed dimer **3*** connects directly to transition structure **10** and **10a**. It exhibits an elongated N-Li bond length of 2.68 Å.

Atom	X	Y	Z	Atom	X	Y	Z
C	3.426237	-0.427821	-0.283587	H	-2.661415	2.227511	2.055561
N	2.226054	0.127897	-0.915322	C	0.350575	0.833835	3.114525
Li	1.622508	1.564067	0.162849	H	1.399906	1.148709	3.125096
N	-0.120884	1.964397	0.951106	H	0.021573	0.722985	4.155878
Li	-0.308638	0.088012	-0.026578	H	0.302686	-0.155569	2.641993
O	-0.435677	-1.839014	0.776563	H	-0.369744	2.810313	2.890739
C	-1.427480	-2.393495	1.670724	C	-0.573651	3.252629	0.397904
C	-0.770552	-3.607574	2.364697	C	0.193298	4.481126	0.948483
C	0.721078	-3.459980	2.008874	H	1.250494	4.434272	0.647165
C	0.649111	-2.783968	0.644914	H	-0.224473	5.420037	0.560314
H	0.409599	-3.509949	-0.146342	H	0.163629	4.537239	2.041060
H	1.525170	-2.211688	0.345647	C	-0.455869	3.277272	-1.130674
H	1.249539	-4.417625	1.980439	H	-0.995206	2.447081	-1.594742
H	1.231265	-2.806526	2.725127	H	-0.848607	4.216070	-1.540265
H	-1.168115	-4.543856	1.957822	H	0.593485	3.205378	-1.449677
H	-0.952249	-3.611655	3.443179	H	-1.643687	3.431267	0.629471
H	-1.706714	-1.606125	2.374813	C	2.159612	-0.196302	-2.339912
H	-2.316943	-2.678012	1.094615	C	1.150637	0.694894	-3.071796
O	-1.945706	-0.146384	-1.199861	H	1.434036	1.749754	-2.993796
C	-3.115434	0.695441	-1.166654	H	1.097255	0.436583	-4.137536
C	-4.284619	-0.280737	-1.244579	H	0.142190	0.585246	-2.652190
C	-3.753779	-1.321543	-2.247285	C	1.828766	-1.679860	-2.638426
C	-2.235334	-1.333774	-1.977165	H	0.815883	-1.926301	-2.292731
H	-1.644960	-1.309614	-2.899047	H	1.881039	-1.893326	-3.714952
H	-1.914173	-2.191116	-1.379561	H	2.526662	-2.360345	-2.137266
H	-3.957711	-0.996249	-3.273208	H	3.128948	-0.005421	-2.836253
H	-4.204737	-2.309712	-2.117551	C	3.413416	-0.137804	1.225285
H	-5.213721	0.195143	-1.572192	H	2.504388	-0.515331	1.704285

Table 1 (continued).

H	-4.459972	-0.736800	-0.263184	H	4.276106	-0.589712	1.728883
H	-3.064186	1.283288	-0.249321	H	3.475144	0.946261	1.422098
H	-3.106721	1.376591	-2.029427	C	4.770895	0.091372	-0.849943
C	-0.516658	1.851211	2.362504	H	4.824409	1.184522	-0.749851
C	-2.012372	1.500443	2.557003	H	5.620395	-0.346518	-0.308723
H	-2.236536	0.510462	2.137138	H	4.902658	-0.151739	-1.908484
H	-2.294660	1.490013	3.618957	H	3.474068	-1.536848	-0.376266



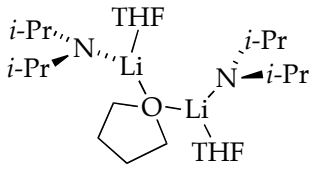


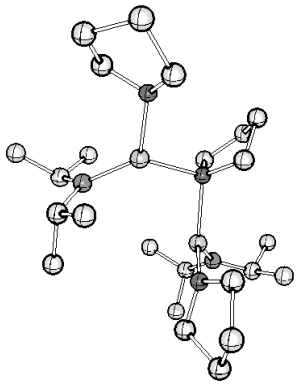
6
G = -996.24738
G_{MP2} = -992.802383
ΔG = 12.2 kcal/mol
ΔG_{MP2} = 5.8 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.739984	0.909518	-1.265496	H	-1.164003	-0.061722	3.517775
N	-1.657323	-0.052568	-1.154433	H	-1.896622	0.279295	1.916956
C	-1.833533	-1.127095	-2.118529	H	-2.678094	-1.975074	1.671695
C	-1.279404	-0.780699	-3.525233	H	-2.920155	-1.771196	3.423456
H	-1.500475	-1.558866	-4.272078	H	-1.314059	-3.818242	2.559507
H	-1.711966	0.159844	-3.885794	H	-0.772838	-2.826939	3.923665
H	-0.190164	-0.642603	-3.483088	H	0.143583	-2.681738	1.022488
C	-1.204481	-2.440764	-1.624950	H	1.081057	-2.355465	2.501384
H	-1.709997	-2.788133	-0.715974	O	1.871871	-0.709018	-0.552973
H	-1.266529	-3.237106	-2.379369	C	2.489283	-1.097627	-1.787877
H	-0.142900	-2.297138	-1.380678	C	3.558661	-2.138193	-1.398840
H	-2.908210	-1.358249	-2.274109	C	3.830863	-1.844085	0.103413
Li	-0.069969	0.062572	-0.073571	C	2.938360	-0.626724	0.400442
O	0.880063	1.846911	0.485875	H	3.490644	0.314030	0.252452
C	1.460351	2.620597	-0.588337	H	2.490727	-0.615830	1.394391
C	1.777282	3.998424	0.003775	H	4.884658	-1.633801	0.310038
C	0.725578	4.123070	1.117527	H	3.535931	-2.696723	0.722644
C	0.645506	2.685461	1.632607	H	4.456600	-2.037535	-2.015796
H	-0.329595	2.424533	2.052500	H	3.178441	-3.154965	-1.532813
H	1.417625	2.484515	2.388915	H	1.705986	-1.476784	-2.444306
H	-0.239679	4.428258	0.699122	H	2.948247	-0.214339	-2.257791
H	1.003569	4.835580	1.900171	C	-4.049821	0.450617	-0.570435
H	1.713385	4.795602	-0.742728	H	-4.349988	-0.545010	-0.916340
H	2.787745	4.014067	0.429880	H	-3.902409	0.392804	0.516912
H	2.345055	2.090753	-0.954720	H	-4.888193	1.136771	-0.764863

Table 1 (continued).

H	0.729062	2.679175	-1.401782	C	-2.345377	2.283546	-0.706302
O	-0.159110	-0.817466	1.856247	H	-1.501094	2.701072	-1.266193
C	0.104092	-2.232042	2.018931	H	-3.178941	2.996739	-0.756210
C	-1.046965	-2.801306	2.862318	H	-2.045679	2.200196	0.348272
C	-2.172958	-1.783175	2.623895	H	-3.014878	1.090871	-2.328091
C	-1.393665	-0.476156	2.524600				



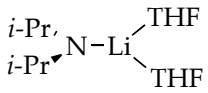


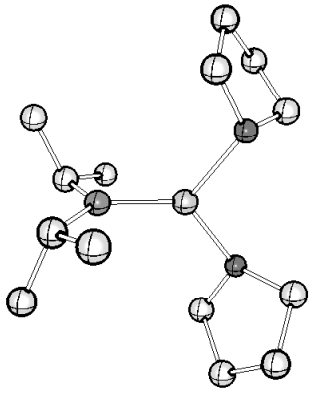
7
G = -1295.446719
G_{MP2} = -1290.87978
ΔG = 23.9 kcal/mol
ΔG_{MP2} = 21.3 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	2.060864	2.473439	-1.765852	C	-2.872929	0.960920	3.788161
N	1.938336	1.736632	-0.518589	C	-2.324099	1.384782	2.427604
Li	1.666746	-0.093941	-0.328202	H	-1.717318	2.294926	2.495470
O	3.237978	-1.345800	-0.034622	H	-3.082897	1.506078	1.650810
C	3.589374	-2.136218	1.124778	H	-3.146158	1.818281	4.410162
C	5.119425	-2.179862	1.164918	H	-3.761352	0.330992	3.663868
C	5.497553	-0.846775	0.502354	H	-0.938489	0.806404	4.773116
C	4.434981	-0.712918	-0.584887	H	-2.011643	-0.554668	5.151680
H	4.716913	-1.251370	-1.498758	H	-1.702852	-1.533320	2.958475
H	4.155462	0.317456	-0.820885	H	-0.101572	-0.768174	3.158069
H	6.512432	-0.841251	0.094159	C	0.075689	-2.586535	0.229869
H	5.413126	-0.022341	1.219755	C	0.504599	-3.629904	-0.793413
H	5.493707	-3.022512	0.571943	C	-0.270112	-3.174859	-2.041317
H	5.502936	-2.285730	2.184161	C	-0.258102	-1.646279	-1.937283
H	3.179860	-1.646274	2.018399	H	-1.218996	-1.181162	-2.180231
H	3.133264	-3.126487	1.024322	H	0.550104	-1.187435	-2.512525
O	0.007401	-1.337172	-0.510561	H	-1.299604	-3.547548	-2.006612
Li	-1.611807	-0.069541	0.069348	H	0.183595	-3.522430	-2.973783
N	-3.174186	-0.025054	-0.966557	H	0.256338	-4.648356	-0.479254
C	-3.527313	1.070667	-1.859809	H	1.585600	-3.567676	-0.961834
H	-4.114750	0.710258	-2.730236	H	0.775197	-2.441391	1.056252
C	-4.397493	2.162424	-1.187185	H	-0.917260	-2.813430	0.638018
H	-5.274739	1.724311	-0.696746	C	2.016163	2.565761	0.670624

Table 1 (continued).

H	-3.814351	2.693578	-0.421969	H	2.951685	3.165963	0.704738
H	-4.759736	2.906484	-1.911496	C	0.861805	3.585447	0.829213
C	-2.265583	1.725732	-2.439141	H	0.813339	4.274971	-0.020151
H	-1.709267	1.020355	-3.067548	H	-0.100355	3.058058	0.880410
H	-2.505146	2.605109	-3.050741	H	0.978314	4.192452	1.738427
H	-1.593069	2.062382	-1.635816	C	2.052008	1.668183	1.918960
C	-4.274882	-0.955291	-0.784461	H	2.900785	0.972044	1.874004
H	-5.244242	-0.424991	-0.669011	H	2.146006	2.252481	2.843173
C	-4.093876	-1.773038	0.504024	H	1.121142	1.084822	1.990682
H	-3.150031	-2.340578	0.467930	H	1.315564	3.292955	-1.842635
H	-4.060303	-1.116952	1.382144	C	1.768897	1.540379	-2.949217
H	-4.902107	-2.501669	0.647883	H	1.870267	2.056600	-3.911983
C	-4.471224	-1.932931	-1.971481	H	2.472434	0.692167	-2.956357
H	-5.376224	-2.547765	-1.857816	H	0.748359	1.146591	-2.885680
H	-4.556982	-1.388900	-2.918618	C	3.440043	3.144053	-1.986967
H	-3.608445	-2.609428	-2.053606	H	3.457615	3.727329	-2.917960
O	-1.454974	0.292328	2.006830	H	3.695376	3.826798	-1.169071
C	-1.179952	-0.581986	3.122820	H	4.233699	2.386024	-2.046569
C	-1.707892	0.141566	4.364230				



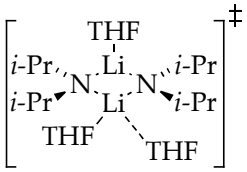


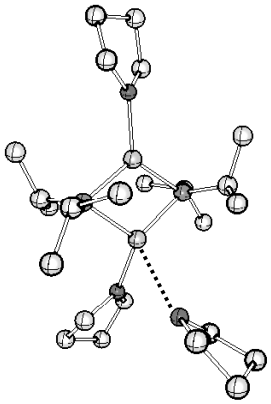
8
G = -763.908312
G_{MP2} = -761.230838
ΔG = 5.5 kcal/mol
ΔG_{MP2} = 6.9 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.620691	2.385888	1.043481	H	-2.159107	-3.421673	-0.578605
N	-0.000631	1.591937	0.000014	H	-1.272626	-2.846301	0.860673
C	0.618888	2.386186	-1.043542	O	1.413260	-1.477861	0.659195
C	1.958906	3.042469	-0.624112	C	1.991867	-2.560094	-0.087797
H	2.355466	3.708145	-1.404656	C	3.307953	-1.991594	-0.615089
H	1.839859	3.638157	0.287930	C	3.786793	-1.111163	0.560966
H	2.712370	2.268506	-0.419421	C	2.490139	-0.769455	1.331869
C	0.857626	1.520629	-2.290915	H	2.217027	0.288157	1.297255
H	-0.089459	1.131338	-2.684603	H	2.532154	-1.106389	2.374607
H	1.358477	2.078589	-3.092423	H	4.299814	-0.210688	0.212422

Table 1 (continued).

H	1.501093	0.660998	-2.042337	H	4.482660	-1.662153	1.202033
H	-0.035053	3.221869	-1.375085	H	3.116481	-1.379208	-1.502798
Li	0.000334	-0.275582	0.000230	H	4.026839	-2.770770	-0.886072
O	-1.412130	-1.478631	-0.658939	H	2.160979	-3.420565	0.577053
C	-1.990341	-2.561735	0.087030	H	1.274211	-2.844220	-0.861655
C	-3.306667	-1.994177	0.614791	C	-1.961165	3.041178	0.623983
C	-3.785699	-1.112530	-0.560323	H	-1.842537	3.636894	-0.288095
C	-2.489268	-0.770669	-1.331575	H	-2.714076	2.266665	0.419339
H	-2.216392	0.287008	-1.297272	H	-2.358211	3.706623	1.404479
H	-2.531435	-1.107918	-2.374215	C	-0.858789	1.520300	2.290956
H	-4.482160	-1.662589	-1.201538	H	0.088586	1.131673	2.684605
H	-4.298113	-0.212135	-0.210681	H	-1.359952	2.078004	3.092448
H	-4.025346	-2.773862	0.884855	H	-1.501704	0.660225	2.042491
H	-3.115447	-1.382724	1.503193	H	0.032667	3.222071	1.374904





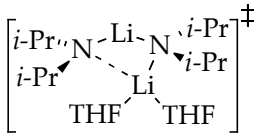
9
G = -1295.468162
G_{MP2} = -1290.908076
$\Delta G^{‡}$ = 10.5 kcal/mol
$\Delta G_{MP2}^{‡}$ = 3.5 kcal/mol

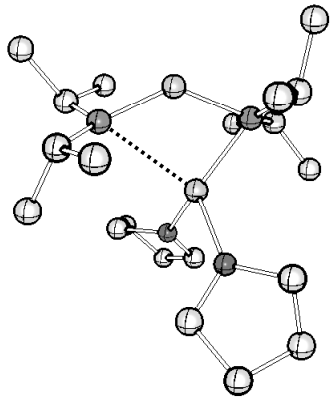
Atom	X	Y	Z	Atom	X	Y	Z
Li	0.681480	0.174041	0.198217	H	-6.631217	0.059755	-1.619163
N	-0.650842	1.368723	-0.958075	H	-6.770071	-0.433149	1.065940
C	-0.938767	2.761153	-0.577105	H	-6.161678	-1.719020	0.008376
C	-0.663346	3.032749	0.906930	H	-4.225903	-1.499955	1.435073
H	0.355904	2.745297	1.183795	H	-4.533239	0.233211	1.709227
H	-0.797575	4.096906	1.140974	C	-0.544731	1.287888	-2.423535
H	-1.355590	2.471288	1.544509	C	-0.730664	-0.144414	-2.936266
C	-2.391874	3.214364	-0.873839	H	-1.689943	-0.567886	-2.609649
H	-3.096699	2.649672	-0.248082	H	-0.710022	-0.179365	-4.033299
H	-2.532809	4.283622	-0.661489	H	0.068692	-0.797100	-2.570578
H	-2.666221	3.054004	-1.922528	C	0.786970	1.833965	-2.996524
H	-0.287308	3.463185	-1.136671	H	1.628277	1.216570	-2.657203
Li	-1.724383	-0.070755	-0.000344	H	0.782861	1.833420	-4.095957
N	-0.531551	-1.302068	1.121228	H	0.972584	2.864897	-2.674726
C	-0.647017	-1.243656	2.585838	H	-1.342650	1.884192	-2.908822
C	0.628763	-1.684037	3.347349	O	2.869745	-0.936722	-1.124503

Table 1 (continued).

H	1.449806	-0.984337	3.151559	C	3.646135	-1.609009	-0.114353
H	0.459550	-1.714046	4.433175	C	4.301360	-2.806484	-0.808790
H	0.962629	-2.681657	3.042535	C	4.482928	-2.279165	-2.240544
C	-1.039932	0.154922	3.073005	C	3.212464	-1.444092	-2.428652
H	-1.991785	0.478955	2.632228	H	2.381898	-2.058750	-2.801380
H	-1.154220	0.178190	4.164337	H	3.342521	-0.594757	-3.106795
H	-0.278638	0.896762	2.805154	H	4.578523	-3.072333	-2.988383
H	-1.449885	-1.918335	2.944964	H	5.374728	-1.643781	-2.304044
C	-0.559356	-2.714548	0.701516	H	3.623949	-3.668220	-0.803150
C	-1.961356	-3.372294	0.776530	H	5.239433	-3.107718	-0.332332
H	-2.642349	-2.891319	0.061205	H	4.402336	-0.913004	0.276971
H	-1.916617	-4.443437	0.534001	H	2.974543	-1.888190	0.702699
H	-2.402796	-3.285389	1.775919	O	2.310950	1.198885	0.992677
C	-0.022406	-2.916933	-0.719466	C	2.960308	2.126151	0.088817
H	0.953883	-2.438124	-0.844310	C	3.681185	3.129572	0.986558
H	0.080833	-3.985963	-0.948159	C	4.092236	2.247765	2.175315
H	-0.704652	-2.493358	-1.464754	C	2.890901	1.305847	2.311764
H	0.092201	-3.326237	1.355116	H	2.131583	1.710716	2.992017
O	-3.695500	-0.248253	-0.125193	H	3.166313	0.305138	2.656035
C	-4.582901	-0.577518	0.971529	H	4.283356	2.811919	3.093112
C	-5.980318	-0.695019	0.355576	H	4.998851	1.680668	1.932152
C	-5.891438	0.266420	-0.839975	H	2.991284	3.916355	1.313278
C	-4.459151	0.037755	-1.320048	H	4.529780	3.605499	0.485646
H	-4.006561	0.904257	-1.805901	H	3.658247	1.564619	-0.543377
H	-4.395675	-0.826311	-1.995116	H	2.185844	2.562806	-0.543316
H	-6.022365	1.303826	-0.510155				

Table 1 (continued).





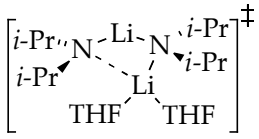
10
G = -1063.11353
G_{MP2} = -1059.322919
$\Delta G^{‡}$ = 13.8 kcal/mol
$\Delta G_{MP2}^{‡}$ = 13.1 kcal/mol

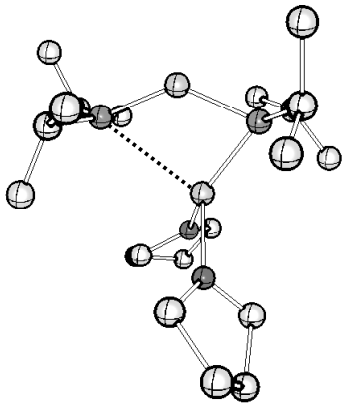
Transition structure **10** connects to disolvated open dimer **4c**.

Atom	X	Y	Z	Atom	X	Y	Z
C	3.446563	-0.423810	-0.280640	H	-2.665936	2.229715	2.058056
N	2.247606	0.128915	-0.915718	C	0.349554	0.840271	3.112913
Li	1.616388	1.551906	0.160785	H	1.398733	1.155763	3.119717
N	-0.130638	1.959457	0.945956	H	0.023489	0.731862	4.155437
Li	-0.345875	0.092097	-0.015986	H	0.301189	-0.150198	2.642720
O	-0.448614	-1.831852	0.780804	H	-0.370224	2.816627	2.881838
C	-1.428123	-2.395050	1.683140	C	-0.580114	3.247231	0.388882
C	-0.754268	-3.602106	2.372894	C	0.198732	4.473355	0.927604
C	0.733578	-3.437862	2.008894	H	1.253275	4.418245	0.618410
C	0.647121	-2.764097	0.644674	H	-0.215706	5.413285	0.538325
H	0.411732	-3.493468	-0.144622	H	0.177765	4.534429	2.020174
H	1.515524	-2.182214	0.340657	C	-0.473836	3.262751	-1.140678
H	1.272562	-4.389543	1.978358	H	-1.021486	2.432959	-1.595876
H	1.240249	-2.778204	2.721934	H	-0.864278	4.201437	-1.552746
H	-1.143765	-4.542450	1.967570	H	0.572572	3.182626	-1.466611
H	-0.930274	-3.608585	3.452318	H	-1.647150	3.433114	0.628054
H	-1.709353	-1.609734	2.388899	C	2.179843	-0.200228	-2.338395
H	-2.319206	-2.688258	1.113945	C	1.167526	0.686922	-3.070420
O	-1.969798	-0.145738	-1.197590	H	1.449027	1.742545	-2.995587
C	-3.145041	0.688736	-1.165455	H	1.111467	0.425970	-4.135382
C	-4.307908	-0.294759	-1.245322	H	0.160324	0.576212	-2.647576
C	-3.769036	-1.332298	-2.247173	C	1.850478	-1.684993	-2.633228
C	-2.251272	-1.336136	-1.973725	H	0.836675	-1.930867	-2.289332
H	-1.658676	-1.310038	-2.894126	H	1.905126	-1.901531	-3.709037
H	-1.926840	-2.190580	-1.373780	H	2.547513	-2.363777	-2.128538
H	-3.972466	-1.007863	-3.273467	H	3.147976	-0.008867	-2.837275
H	-4.214682	-2.323006	-2.118615	C	3.434129	-0.120826	1.225742
H	-5.239281	0.175554	-1.574507	H	2.524711	-0.493758	1.708025
H	-4.482188	-0.751972	-0.264266	H	4.296205	-0.569217	1.733548

Table 1 (continued).

H	-3.098885	1.276561	-0.247723	H	3.496507	0.965015	1.412098
H	-3.139229	1.370401	-2.027781	C	4.792337	0.087357	-0.851507
C	-0.520374	1.854576	2.359886	H	4.849560	1.180918	-0.758841
C	-2.015580	1.506161	2.562919	H	5.640806	-0.349924	-0.308135
H	-2.242463	0.512722	2.152344	H	4.922077	-0.163469	-1.908572
H	-2.293703	1.504407	3.626005	H	3.491860	-1.533894	-0.363855





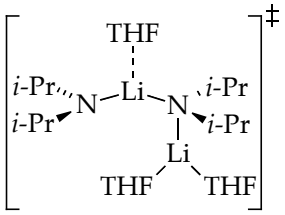
10*
G = -1063.113154
G_{MP2} = -1059.321215
$\Delta G^{‡}$ = 14.0 kcal/mol
$\Delta G_{MP2}^{‡}$ = 14.2 kcal/mol

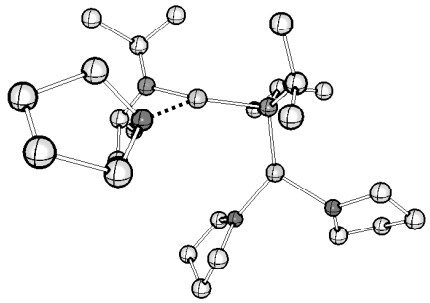
10* is akin to **10** with an activation barrier of 1.1 kcal/mol higher. **10*** connects to disolvated open dimer **4b**.

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.114283	-0.542780	-2.472623	H	2.288305	-2.294138	-0.238505
N	-2.200964	-0.293521	-1.035316	C	-0.282290	-4.291674	0.977752
Li	-1.638272	-1.556364	0.252300	H	-0.890476	-4.324505	1.889516
N	0.024066	-1.819164	1.300307	H	0.233957	-5.257738	0.884766
Li	0.388083	-0.083821	0.240418	H	-0.965282	-4.200001	0.119441
O	2.072738	0.239915	-0.892168	H	1.428184	-3.325858	1.817244
C	3.261165	0.603800	-0.151312	C	-0.082042	-1.666733	2.761898
C	4.348374	0.831190	-1.202036	C	-1.281619	-0.802666	3.166746
C	3.948491	-0.174272	-2.292622	H	-1.231794	0.189120	2.702926
C	2.420294	-0.099491	-2.256453	H	-1.326207	-0.659566	4.253863
H	2.035877	0.686941	-2.917066	H	-2.226593	-1.269035	2.856821
H	1.930307	-1.041724	-2.512055	C	1.206916	-1.100943	3.402358
H	4.352575	0.071261	-3.279127	H	2.080060	-1.698413	3.115893
H	4.289488	-1.181344	-2.026476	H	1.154758	-1.091156	4.500409
H	4.301338	1.856250	-1.588800	H	1.382371	-0.071455	3.061788
H	5.353639	0.663265	-0.804409	H	-0.249800	-2.653205	3.235094
H	3.519155	-0.220532	0.526153	C	-3.281174	0.647639	-0.736740
H	3.024419	1.488129	0.445189	C	-4.700528	0.049387	-0.904190
O	0.413563	1.897745	0.836375	H	-4.854287	-0.369084	-1.904205
C	0.398198	2.619552	2.090225	H	-5.481463	0.805705	-0.740931

Table 1 (continued).

C	0.459327	4.101778	1.717075	H	-4.851788	-0.761377	-0.177794
C	-0.281521	4.120853	0.370978	C	-3.164962	1.195338	0.690502
C	0.185116	2.813361	-0.268107	H	-3.311295	0.394958	1.427899
H	-0.547405	2.350766	-0.933274	H	-3.927226	1.959798	0.888526
H	1.130614	2.942119	-0.810068	H	-2.176396	1.631489	0.864879
H	-1.365189	4.102015	0.530863	H	-3.240444	1.530761	-1.409910
H	-0.041695	4.993317	-0.244035	C	-1.408090	0.587957	-3.260248
H	-0.001326	4.739965	2.476895	H	-1.881734	1.558209	-3.070316
H	1.499505	4.424370	1.587253	H	-1.438966	0.414754	-4.345536
H	1.246394	2.280725	2.691934	H	-0.355687	0.663269	-2.956243
H	-0.528199	2.378040	2.624589	C	-1.411238	-1.873215	-2.764648
C	0.702231	-3.098732	1.014834	H	-0.385898	-1.861259	-2.373766
C	1.519298	-3.072058	-0.281924	H	-1.349072	-2.075484	-3.841551
H	0.879417	-2.871123	-1.149099	H	-1.944631	-2.709598	-2.293709
H	2.012532	-4.036740	-0.457922	H	-3.121579	-0.633572	-2.922681





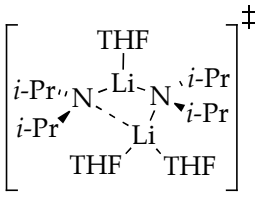
11
G = -1295.456439
G_{MP2} = -1290.890247
$\Delta G^{‡}$ = 17.8 kcal/mol
$\Delta G_{MP2}^{‡}$ = 14.7 kcal/mol

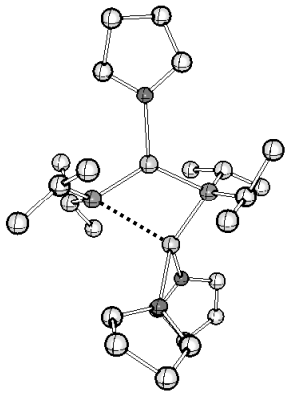
Atom	X	Y	Z	Atom	X	Y	Z
C	-0.892566	-2.419404	-1.171013	H	4.082729	1.184968	-1.847740
N	-0.661285	-1.593854	0.029333	C	2.346574	2.003749	-0.933718
Li	-1.814919	-0.025294	0.022911	H	1.262974	1.823752	-0.862909
O	-3.729470	0.035294	0.562338	H	2.752197	1.946280	0.080913
C	-4.727749	0.741847	-0.207108	H	2.495344	3.023821	-1.315207
C	-5.932414	-0.194667	-0.258306	C	2.520846	1.191731	-3.303075
C	-5.871909	-0.856281	1.127320	H	2.816626	2.184339	-3.675030
C	-4.364051	-1.001906	1.363528	H	2.941291	0.446233	-3.986676
H	-3.978733	-1.966338	1.021414	H	1.426275	1.110980	-3.366576
H	-4.073704	-0.856112	2.407565	C	-0.750886	-2.356191	1.283959
H	-6.389191	-1.818975	1.167454	H	-1.698301	-2.929760	1.339500
H	-6.320960	-0.200304	1.882042	C	0.378222	-3.391448	1.487088
H	-5.798705	-0.942172	-1.048598	H	0.429639	-4.101444	0.654900
H	-6.869810	0.337804	-0.444135	H	1.353965	-2.891741	1.561007
H	-4.973144	1.685623	0.299059	H	0.228394	-3.971018	2.408242

Table 1 (continued).

H	-4.298662	0.970105	-1.186013	C	-0.763976	-1.393273	2.482179
O	-1.589021	1.844997	-0.556654	H	-1.600147	-0.680470	2.418432
C	-1.476342	2.917015	0.410886	H	-0.877820	-1.938783	3.427914
C	-1.703213	4.202564	-0.383087	H	0.168873	-0.821274	2.527910
C	-1.086167	3.844935	-1.744583	H	-0.132781	-3.219912	-1.264654
C	-1.467237	2.371316	-1.905894	C	-0.747897	-1.546458	-2.427117
H	-0.717068	1.782594	-2.438196	H	-0.863831	-2.142970	-3.340596
H	-2.437661	2.252980	-2.405557	H	-1.527143	-0.766208	-2.452204
H	0.002752	3.950036	-1.708963	H	0.232464	-1.055697	-2.461154
H	-1.463874	4.461034	-2.565605	C	-2.262164	-3.136624	-1.227060
H	-1.233547	5.070368	0.088934	H	-2.359090	-3.718538	-2.152697
H	-2.775845	4.407225	-0.484256	H	-2.408046	-3.830281	-0.392011
H	-2.219145	2.740308	1.194682	H	-3.082696	-2.403348	-1.204725
H	-0.473163	2.886529	0.853010	O	2.130157	0.351341	2.166802
Li	1.230999	-0.793283	-0.235581	C	1.976652	1.475563	3.044284
N	2.722385	-0.381693	-1.341487	C	3.306087	1.626723	3.796645
C	3.590441	-1.391590	-1.925789	C	4.308659	1.044417	2.787290
H	3.653697	-1.295202	-3.032095	C	3.503519	-0.099089	2.169231
C	5.055745	-1.343674	-1.420719	H	3.578883	-1.011831	2.779350
H	5.489329	-0.343616	-1.535680	H	3.761520	-0.327781	1.131310
H	5.099997	-1.607279	-0.355208	H	5.240265	0.703397	3.249435
H	5.698771	-2.046413	-1.970431	H	4.559820	1.789356	2.022935
C	3.028077	-2.795087	-1.659973	H	3.297539	1.026287	4.714299
H	2.036078	-2.913361	-2.110738	H	3.514965	2.664923	4.074283
H	3.681524	-3.579503	-2.063530	H	1.759210	2.370434	2.441960
H	2.932611	-2.970391	-0.578165	H	1.123748	1.293825	3.709797
C	2.995467	0.950668	-1.845601				

Table 1 (Continued).



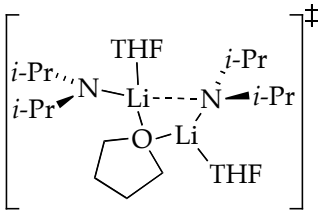


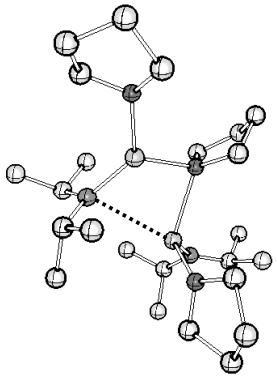
12
G = -1295.456449
G_{MP2} = -1290.897348
$\Delta G^{‡}$ = 17.8 kcal/mol
$\Delta G_{MP2}^{‡}$ = 10.3 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	0.636461	1.802019	-2.288673	C	1.392000	-2.317572	2.901757
N	0.822011	1.650311	-0.845433	H	2.284188	-1.691893	2.772302
Li	1.509939	-0.037022	-0.014373	H	1.205622	-2.416944	3.979311
N	0.286781	-1.501106	0.742168	H	1.623810	-3.316002	2.517617
Li	-1.146230	-0.270797	-0.032281	C	-0.077981	-0.320020	2.884625
O	-2.510661	1.057607	0.794776	H	-0.890699	0.233692	2.405983
C	-2.337956	2.465455	0.532152	H	-0.334522	-0.458221	3.943108
C	-2.432389	3.108190	1.912554	H	0.816931	0.312346	2.839767
C	-3.519611	2.258037	2.608278	H	-0.692228	-2.316303	2.459782
C	-3.489760	0.913150	1.840339	O	3.539508	-0.424249	-0.080401
H	-3.182299	0.065610	2.458766	C	4.465644	0.420610	-0.807038
H	-4.466721	0.683652	1.395180	C	5.845577	0.108709	-0.229752
H	-3.319955	2.124170	3.675140	C	5.707807	-1.380081	0.120532
H	-4.503762	2.728962	2.513868	C	4.268910	-1.449874	0.635618
H	-1.472274	3.009721	2.429465	H	3.779447	-2.410189	0.455585
H	-2.689185	4.170776	1.868346	H	4.219378	-1.228689	1.708550
H	-3.147604	2.816828	-0.128143	H	5.826596	-1.996423	-0.778642
H	-1.372289	2.558508	0.028097	H	6.432293	-1.723139	0.865379
O	-2.826029	-1.121251	-1.159407	H	6.651578	0.317555	-0.939656
C	-3.370205	-2.445604	-0.949735	H	6.026795	0.699619	0.676360
C	-4.859373	-2.384226	-1.339020	H	4.149812	1.457471	-0.677231
C	-5.158347	-0.876746	-1.333203	H	4.409965	0.168246	-1.872591
C	-3.822443	-0.297125	-1.791052	C	1.578011	2.774401	-0.291109
H	-3.714339	-0.353768	-2.883831	C	1.976020	2.495264	1.167560
H	-3.649180	0.730217	-1.469606	H	2.604451	1.599818	1.261741
H	-5.991110	-0.597334	-1.985685	H	2.538744	3.334121	1.596772
H	-5.387610	-0.532409	-0.318163	H	1.079821	2.343049	1.781508
H	-5.013832	-2.797044	-2.341993	C	0.875046	4.159259	-0.322210
H	-5.488963	-2.950056	-0.645975	H	0.035927	4.191469	0.384163
H	-3.223505	-2.695854	0.105007	H	1.574962	4.957822	-0.038812
H	-2.809624	-3.164728	-1.555670	H	0.487522	4.405706	-1.316147
C	0.657291	-2.754042	0.069113	H	2.533919	2.936276	-0.843762

Table 1 (Continued).

C	-0.228490	-3.982087	0.385700	C	-0.555892	0.969153	-2.774494
H	-1.269985	-3.797777	0.102697	H	-1.479919	1.305108	-2.290136
H	0.122300	-4.863948	-0.166914	H	-0.697773	1.050809	-3.860567
H	-0.216642	-4.238917	1.449715	H	-0.412035	-0.094191	-2.545512
C	0.690582	-2.553474	-1.453263	C	1.880444	1.442510	-3.140188
H	1.362710	-1.735653	-1.742380	H	2.121643	0.375543	-3.036146
H	1.043009	-3.459209	-1.963223	H	1.720468	1.649978	-4.208251
H	-0.308431	-2.317014	-1.841562	H	2.756911	2.019299	-2.824130
H	1.685699	-3.068606	0.349498	H	0.391623	2.848661	-2.556343
C	0.174180	-1.670666	2.199914				





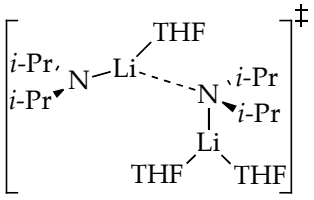
13
G = -1295.443878
G_{MP2} = -1290.879859
$\Delta G^{‡}$ = 25.7 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 21.2 kcal/mol

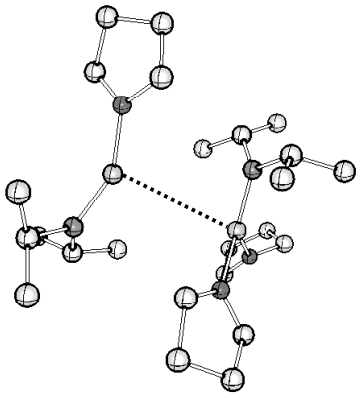
13 connects to trisolvated open dimer **5a** and **7**.

Atom	X	Y	Z	Atom	X	Y	Z
C	1.323554	2.622040	-1.440307	C	-3.012289	-0.033052	3.811668
N	1.335446	1.768721	-0.254470	C	-2.491226	0.754934	2.609980
Li	1.732490	-0.056325	-0.368838	H	-2.054362	1.714114	2.912435
O	3.543874	-0.882754	-0.243906	H	-3.229163	0.922319	1.822343
C	4.062073	-1.902955	0.641902	H	-3.427126	0.618789	4.586220
C	5.572265	-1.663028	0.730819	H	-3.794879	-0.735034	3.501547
C	5.676126	-0.149143	0.487613	H	-1.106800	-0.141595	4.859219
C	4.592355	0.078021	-0.562663	H	-1.981233	-1.685767	4.863315
H	4.958868	-0.133474	-1.575284	H	-1.492323	-2.077211	2.520885
H	4.130293	1.067240	-0.539900	H	-0.005613	-1.208559	2.993359
H	6.664578	0.164337	0.139710	C	0.488202	-2.757957	-0.013584
H	5.443362	0.405901	1.403717	C	0.731434	-3.767642	-1.130455
H	6.094360	-2.213674	-0.060215	C	-0.167780	-3.214308	-2.247300
H	5.985395	-1.979227	1.693118	C	-0.028934	-1.699086	-2.088230
H	3.579212	-1.789143	1.621524	H	-0.955520	-1.140680	-2.261225
H	3.804052	-2.885023	0.232957	H	0.780918	-1.294252	-2.703052
O	0.343476	-1.476376	-0.676978	H	-1.206550	-3.521568	-2.086704
Li	-1.293114	0.191871	-0.001682	H	0.132838	-3.548313	-3.244556
N	-2.923400	0.103986	-0.998597	H	0.473582	-4.788342	-0.831721

Table 1 (Continued).

C	-3.492009	1.285101	-1.641593	H	1.784568	-3.753485	-1.436961
H	-4.131638	1.004834	-2.503402	H	1.309129	-2.674586	0.703880
C	-4.400008	2.121808	-0.703619	H	-0.436467	-2.980388	0.530738
H	-5.160785	1.492494	-0.226038	C	1.488262	2.500248	0.995318
H	-3.799264	2.587984	0.089807	H	2.394529	3.141252	0.986715
H	-4.925333	2.924292	-1.242310	C	0.314420	3.447140	1.336509
C	-2.391519	2.188224	-2.208780	H	0.158350	4.192408	0.548721
H	-1.832506	1.671576	-2.996512	H	-0.618245	2.877053	1.437949
H	-2.800644	3.116303	-2.630021	H	0.491423	3.991789	2.274818
H	-1.678546	2.470267	-1.422054	C	1.694764	1.511463	2.153077
C	-3.894920	-0.978674	-0.970880	H	2.573486	0.875803	1.968793
H	-4.908306	-0.607225	-0.702797	H	1.856357	2.029398	3.107140
C	-3.547424	-2.023948	0.099388	H	0.812450	0.869177	2.262069
H	-2.544185	-2.437859	-0.079332	H	0.422601	3.268166	-1.479917
H	-3.550460	-1.576807	1.099142	C	1.264443	1.743099	-2.696782
H	-4.254588	-2.863774	0.094268	H	1.193402	2.344081	-3.611540
C	-4.072361	-1.703423	-2.331460	H	2.172654	1.123886	-2.780027
H	-4.894361	-2.434254	-2.305038	H	0.392426	1.082651	-2.665794
H	-4.290364	-0.990590	-3.134022	C	2.524745	3.589064	-1.579468
H	-3.152337	-2.237295	-2.606238	H	2.452718	4.164915	-2.511441
O	-1.431897	-0.061762	2.035417	H	2.576958	4.309467	-0.756517
C	-1.096785	-1.138797	2.931537	H	3.474113	3.034828	-1.597653
C	-1.758571	-0.795071	4.267754				





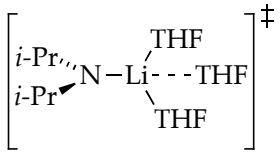
14
G = -1295.449326
G_{MP2} = -1290.877105
$\Delta G^{‡}$ = 22.3 kcal/mol
$\Delta G_{MP2}^{‡}$ = 23.0 kcal/mol

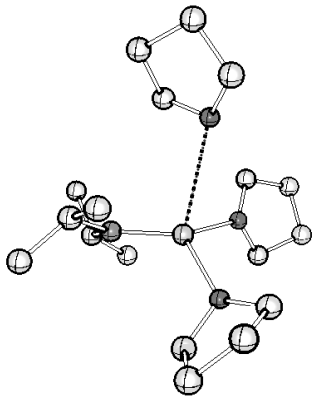
Atom	X	Y	Z	Atom	X	Y	Z
C	1.998047	-2.440567	1.794156	H	-5.307965	-0.331767	0.325113
N	2.597024	-1.667569	0.720492	H	-4.239966	1.092047	0.139970
Li	2.253942	0.099387	0.331597	C	-1.083484	2.749563	0.267657
O	2.798805	1.907549	0.160525	C	-2.286546	3.702730	0.500577
C	3.596110	2.622805	1.137194	H	-3.181195	3.138427	0.797732
C	4.004805	3.927200	0.451212	H	-2.067548	4.436533	1.290003
C	2.814595	4.186622	-0.486461	H	-2.532406	4.264777	-0.405909

Table 1 (continued).

C	2.459154	2.777163	-0.955734	C	-0.703776	2.106274	1.610442
H	1.400680	2.626251	-1.174614	H	0.210430	1.508748	1.508255
H	3.062815	2.473831	-1.820858	H	-0.536428	2.856716	2.393657
H	1.974986	4.622928	0.066035	H	-1.502502	1.436699	1.958447
H	3.058061	4.851435	-1.320296	H	-0.242736	3.436500	0.004067
H	4.176077	4.735048	1.168690	C	-1.356089	2.250631	-2.097705
H	4.925151	3.783779	-0.126933	C	-0.610623	1.347453	-3.101344
H	4.438994	1.986329	1.420906	H	-1.030563	0.332678	-3.075100
H	2.974619	2.806838	2.022167	H	-0.696806	1.715443	-4.132732
N	-1.245827	1.724573	-0.743670	H	0.453204	1.268715	-2.849725
Li	-1.718222	-0.075010	-0.386750	C	-2.812049	2.416777	-2.609699
O	-1.343436	-1.812615	-1.241548	H	-3.406367	3.045259	-1.940900
C	-2.388815	-2.767475	-1.539990	H	-2.850910	2.859948	-3.615897
C	-1.776508	-3.762833	-2.528083	H	-3.301501	1.432983	-2.660008
C	-0.293922	-3.742903	-2.126949	H	-0.883428	3.254537	-2.162195
C	-0.073274	-2.269730	-1.792301	C	3.779414	-2.292483	0.146704
H	0.709032	-2.091370	-1.046473	C	4.584309	-1.257681	-0.655042
H	0.140518	-1.680431	-2.692647	H	4.923837	-0.438645	-0.007548
H	-0.123837	-4.365250	-1.240745	H	5.467294	-1.702042	-1.131043
H	0.373953	-4.092912	-2.919160	H	3.964659	-0.828124	-1.458429
H	-2.236843	-4.753100	-2.456690	C	3.475723	-3.505478	-0.766721
H	-1.898301	-3.404771	-3.557259	H	2.940900	-3.179989	-1.669081
H	-3.251434	-2.226191	-1.940535	H	4.395678	-4.016968	-1.083558
H	-2.688886	-3.259844	-0.606650	H	2.849787	-4.243697	-0.252317
O	-3.293908	-0.617086	0.735168	H	4.466308	-2.668062	0.933125
C	-4.463548	0.222651	0.760167	C	0.581794	-1.921058	2.086352
C	-4.708315	0.542008	2.247373	H	-0.054602	-2.002832	1.196914
C	-3.935206	-0.572849	3.006501	H	0.107715	-2.475530	2.907521
C	-3.390356	-1.472232	1.884782	H	0.616481	-0.862253	2.384633
H	-2.396985	-1.882114	2.076383	C	2.812960	-2.427484	3.111071
H	-4.082621	-2.298466	1.663307	H	2.856045	-1.407383	3.516514
H	-3.111371	-0.144585	3.584534	H	2.368762	-3.083373	3.873731
H	-4.571267	-1.133158	3.698051	H	3.842666	-2.764098	2.947767
H	-4.311158	1.528683	2.500369	H	1.882263	-3.510708	1.517365
H	-5.776931	0.542976	2.481639				

Table 1 (continued).



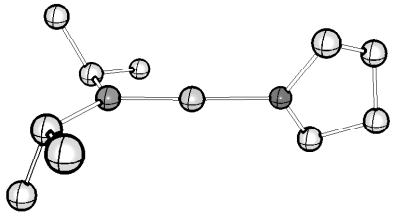


15
G = -1296.24815
G_{MP2} = -992.798680
$\Delta G^{‡}$ = 11.5 kcal/mol
$\Delta G_{MP2}{}^{‡}$ = 8.2 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.151278	-1.488130	2.681120	H	3.534626	0.770454	0.435262
N	-0.164812	-1.467352	1.228815	H	2.341117	-0.557186	0.535425
C	0.289774	-2.702771	0.617291	H	3.556732	-1.859054	-1.133666
C	-0.554367	-3.958282	0.954354	H	4.926531	-1.075433	-0.323320
H	-0.157509	-4.852688	0.453927	H	4.609788	-0.661881	-3.012863
H	-0.569410	-4.166906	2.029467	H	4.967456	0.732112	-1.979283
H	-1.594842	-3.815643	0.630561	H	2.254370	-0.132925	-3.084187
C	0.323031	-2.542990	-0.911898	H	2.881816	1.518747	-2.882406
H	0.907172	-1.660955	-1.201427	O	-2.248196	0.188575	-0.846609
H	0.759633	-3.422584	-1.402999	C	-3.234348	-0.822364	-0.532791
H	-0.694912	-2.416193	-1.305210	C	-3.575297	-1.523313	-1.869268
H	1.332811	-2.964970	0.914553	C	-2.810512	-0.703413	-2.939124
Li	-0.558478	0.108232	0.258241	C	-2.469075	0.594479	-2.202232
O	-0.419617	2.091348	0.531713	H	-3.303905	1.311694	-2.244023
C	-1.528275	2.884759	0.977565	H	-1.559794	1.089559	-2.552220
C	-1.155259	4.308241	0.559893	H	-3.399667	-0.527226	-3.844342
C	0.382221	4.333202	0.751116	H	-1.888303	-1.216883	-3.227861
C	0.778601	2.837743	0.830021	H	-4.654711	-1.508309	-2.050148
H	1.123496	2.569130	1.837427	H	-3.255768	-2.568918	-1.866618
H	1.524773	2.524932	0.099640	H	-2.768500	-1.466245	0.217071
H	0.661562	4.855185	1.671561	H	-4.117147	-0.330150	-0.102241
H	0.880672	4.842997	-0.078311	C	1.263601	-1.519934	3.312832
H	-1.671536	5.068479	1.153794	H	1.849168	-2.368466	2.940322
H	-1.415432	4.466219	-0.492012	H	1.812534	-0.600820	3.063866
H	-2.424665	2.485055	0.501138	H	1.220519	-1.606365	4.408092
H	-1.631164	2.797571	2.069851	C	-0.910680	-0.270606	3.230384
O	2.194327	0.607162	-1.151787	H	-1.945986	-0.265476	2.865314
C	2.848085	0.520148	-2.429637	H	-0.934774	-0.264849	4.327737
C	4.242371	-0.068381	-2.169853	H	-0.428900	0.662616	2.904118
C	4.010089	-0.891063	-0.892353	H	-0.680027	-2.374855	3.090282
C	3.012848	-0.013937	-0.135625				

Table 1 (continued).

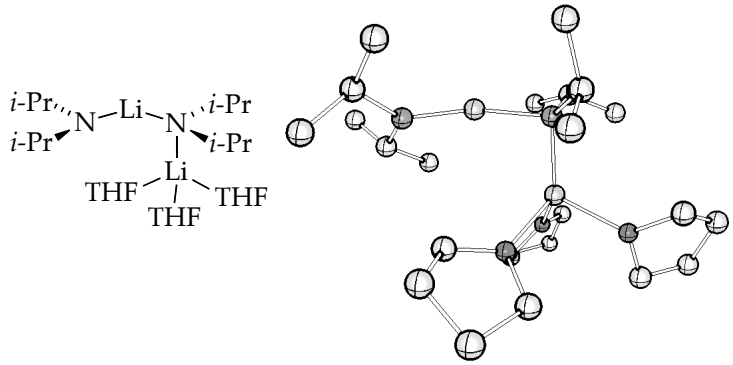
i-Pr, *i*-Pr N−Li−THF



22
G = -531.551232
G_{MP2} = -529.642356
ΔG = 10.4 kcal/mol
ΔG_{MP2} = 18.5 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.542016	-1.124853	0.250648	H	2.348220	0.847909	1.782018
N	-1.666846	0.004061	0.002239	H	2.953005	-0.829438	1.799181
C	-2.347484	1.254768	-0.269229	H	4.171030	1.585096	0.352865
C	-3.002258	1.892262	0.979568	H	5.025029	0.361788	1.312920
H	-3.563807	2.803268	0.727864	H	4.984644	0.062548	-1.400140
H	-3.699608	1.197636	1.460887	H	4.637452	-1.356151	-0.396787
H	-2.230547	2.152542	1.716673	H	2.572887	-1.309176	-1.639343
C	-1.354616	2.254059	-0.882670	H	2.633325	0.462262	-1.824460
H	-0.942280	1.862185	-1.821529	C	-3.253018	-1.653647	-1.017922
H	-1.817755	3.226836	-1.089789	H	-3.822425	-0.860096	-1.514469
H	-0.519867	2.436123	-0.185054	H	-2.510845	-2.028944	-1.735526
H	-3.159095	1.129283	-1.016311	H	-3.954099	-2.467622	-0.784649
Li	0.132813	-0.150494	0.030515	C	-1.733812	-2.265670	0.887470
O	2.027530	-0.218284	0.039331	H	-1.294202	-1.943228	1.840256
C	2.852175	-0.372488	-1.148827	H	-2.347080	-3.155729	1.075181
C	4.299749	-0.345252	-0.651568	H	-0.916615	-2.574689	0.213877
C	4.198913	0.521169	0.614276	H	-3.344540	-0.873878	0.975655
C	2.856769	0.079785	1.193057				

Table 1 (continued).

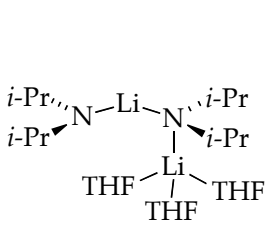


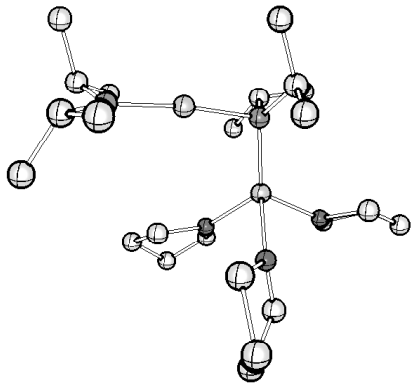
16a
G = -1295.463164
G_{MP2} = -1290.903012
ΔG = 13.6 kcal/mol
ΔG_{MP2} = 6.7 kcal/mol
(connects to **17** and **19**)

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.419882	-1.357612	-2.656833	C	-0.059261	-2.879802	-0.796816
N	0.007859	-1.480905	-1.252086	H	-1.049885	-3.328115	-1.027954
Li	-0.967793	-0.190969	0.041045	C	0.979294	-3.826638	-1.446847
O	-1.559414	1.812365	-0.416194	H	0.922741	-3.812112	-2.540247
C	-1.141011	2.944334	0.385608	H	1.998910	-3.541124	-1.160078
C	-1.474608	4.183768	-0.443846	H	0.820464	-4.865587	-1.127027
C	-2.727135	3.728762	-1.206616	C	0.104037	-2.956400	0.728523
C	-2.397716	2.264841	-1.506760	H	-0.699382	-2.423937	1.250158
H	-1.840935	2.160477	-2.444436	H	0.099280	-3.996670	1.076909
H	-3.278316	1.616817	-1.553279	H	1.055051	-2.504025	1.038087
H	-2.917147	4.305602	-2.116445	Li	1.858727	-0.720368	-1.047479
H	-3.614625	3.804434	-0.566181	N	3.423937	0.163316	-0.519878
H	-0.659023	4.402150	-1.142407	C	3.618687	1.599841	-0.603587
H	-1.640044	5.069742	0.176386	H	3.742152	2.068218	0.402678
H	-1.697281	2.928862	1.332618	C	4.848973	2.061099	-1.422632
H	-0.077660	2.836723	0.601595	H	5.792803	1.734606	-0.973617
O	-2.890402	-0.757288	0.689826	H	4.800131	1.647460	-2.438844
C	-3.914984	0.110914	1.192887	H	4.885056	3.156880	-1.494674
C	-5.208307	-0.308479	0.465178	C	2.372052	2.251968	-1.219636
C	-4.908229	-1.754234	-0.019802	H	1.460703	1.923785	-0.703138
C	-3.511426	-2.046315	0.550448	H	2.418819	3.348003	-1.165007
H	-2.874646	-2.649366	-0.095693	H	2.273969	1.970135	-2.275935
H	-3.575822	-2.523969	1.539973	C	4.587156	-0.559568	-0.027275
H	-4.888086	-1.798681	-1.112277	H	5.491823	-0.339819	-0.629738
H	-5.647873	-2.479731	0.331040	C	4.363554	-2.070990	-0.164548
H	-5.412606	0.350831	-0.383645	H	3.506387	-2.395333	0.443765
H	-6.072937	-0.260918	1.133824	H	4.164101	-2.338407	-1.210325
H	-4.010678	-0.032926	2.279677	H	5.237862	-2.643639	0.170284
H	-3.595194	1.134769	0.997107	C	4.972857	-0.241624	1.438969
O	-0.155676	0.315433	1.889374	H	5.894119	-0.762144	1.735619
C	-0.869759	0.042791	3.116779	H	5.139708	0.831478	1.588470
C	0.166948	0.084692	4.256045	H	4.171736	-0.554422	2.122444
C	1.507981	-0.023285	3.511494	H	-0.016907	-2.186153	-3.266887

Table 1 (continued).

C	1.204652	0.708800	2.210500	C	0.142651	-0.071344	-3.278706
H	1.855632	0.437406	1.369327	H	-0.242396	0.090300	-4.293676
H	1.237559	1.799163	2.357789	H	-0.119899	0.803379	-2.671212
H	1.756358	-1.069722	3.301497	H	1.237996	-0.106701	-3.346887
H	2.342259	0.422597	4.060327	C	-1.953399	-1.408592	-2.857409
H	0.010769	-0.717561	4.983516	H	-2.224013	-1.379207	-3.921940
H	0.107645	1.037628	4.794107	H	-2.375769	-2.330171	-2.440197
H	-1.661041	0.791212	3.249780	H	-2.442392	-0.560919	-2.359821
H	-1.339677	-0.939813	3.012890				





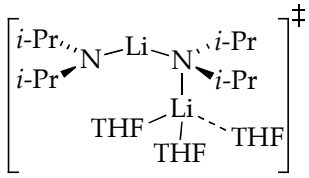
16b
G = -1295.461765
G_{MP2} = -1290.900028
ΔG = 14.5 kcal/mol
ΔG_{MP2} = 8.6 kcal/mol
(conformer of **16a**)

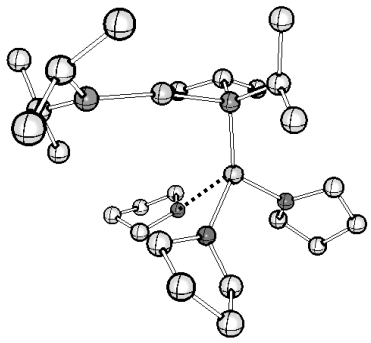
Atom	X	Y	Z	Atom	X	Y	Z
C	0.058653	-2.840247	0.529819	C	0.226125	-2.335610	-1.853985
N	0.048315	-1.783627	-0.500335	H	1.176172	-2.901727	-1.932187
Li	1.071773	-0.102961	0.012533	C	-0.885013	-3.314988	-2.303392
O	0.420576	1.090912	1.603882	H	-0.966133	-4.178688	-1.634682
C	-0.790472	1.889266	1.457377	H	-1.865642	-2.816995	-2.319954
C	-1.192580	2.292638	2.876184	H	-0.690217	-3.699128	-3.313464
C	0.159450	2.340228	3.602735	C	0.334997	-1.203386	-2.882278
C	0.895256	1.161799	2.964028	H	1.168725	-0.533561	-2.641852
H	0.658437	0.220564	3.476055	H	0.500276	-1.600721	-3.891533
H	1.983312	1.283876	2.941953	H	-0.584748	-0.604605	-2.909766
H	0.075899	2.238557	4.689051	Li	-1.822113	-1.037405	-0.417823
H	0.680232	3.281514	3.387979	N	-3.473373	-0.193229	-0.198210
H	-1.839145	1.526214	3.318432	C	-4.051478	0.755066	-1.136633
H	-1.732529	3.243549	2.899260	H	-5.074668	0.451494	-1.440696
H	-0.542985	2.766123	0.844365	C	-4.191755	2.189825	-0.565565
H	-1.554839	1.292172	0.945166	H	-4.727249	2.181864	0.390684
O	1.430489	1.670399	-1.175791	H	-3.199957	2.629221	-0.388958
C	2.362033	2.611417	-0.590235	H	-4.740531	2.855156	-1.248484
C	2.031595	3.981378	-1.195496	C	-3.229531	0.810435	-2.431485

Table 1 (continued).

C	1.396825	3.601463	-2.541374	H	-3.218795	-0.167767	-2.927357
C	0.618701	2.342033	-2.167343	H	-3.622761	1.551838	-3.139711
H	0.461461	1.651101	-2.997124	H	-2.189110	1.090089	-2.208639
H	-0.356815	2.590299	-1.729510	C	-4.455284	-0.658590	0.770546
H	2.171402	3.367146	-3.281413	H	-5.090688	0.176118	1.136885
H	0.753979	4.383741	-2.955458	C	-3.765713	-1.241244	2.011886
H	2.917509	4.615893	-1.294714	H	-3.127913	-2.094005	1.735828
H	1.304517	4.514418	-0.571654	H	-3.132270	-0.488318	2.497196
H	2.246530	2.576077	0.495823	H	-4.492580	-1.606775	2.748846
H	3.379106	2.290641	-0.845179	C	-5.429750	-1.719169	0.199845
O	3.123998	-0.355655	0.281821	H	-6.219035	-1.985464	0.918402
C	3.884319	-0.698166	1.462459	H	-5.919968	-1.356966	-0.710585
C	5.036776	-1.587981	0.984951	H	-4.877485	-2.632210	-0.061380
C	5.247152	-1.102524	-0.457405	H	-0.837661	-3.493070	0.452214
C	3.813156	-0.820606	-0.904353	C	0.002821	-2.217016	1.931634
H	3.313168	-1.725458	-1.269264	H	-0.156421	-2.985811	2.697810
H	3.728498	-0.039979	-1.664952	H	0.946923	-1.706678	2.165014
H	5.744968	-1.840476	-1.093202	H	-0.803680	-1.481984	2.018998
H	5.843084	-0.181971	-0.470974	C	1.267745	-3.803060	0.483850
H	4.733115	-2.640762	0.990469	H	1.237190	-4.501783	1.329804
H	5.927155	-1.487541	1.612590	H	1.294522	-4.403056	-0.431182
H	4.252285	0.230125	1.919222	H	2.207542	-3.236852	0.541549
H	3.219570	-1.199362	2.172042				

Table 1 (continued).



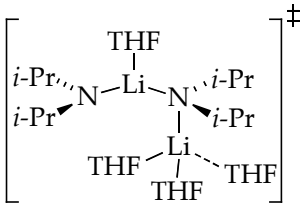


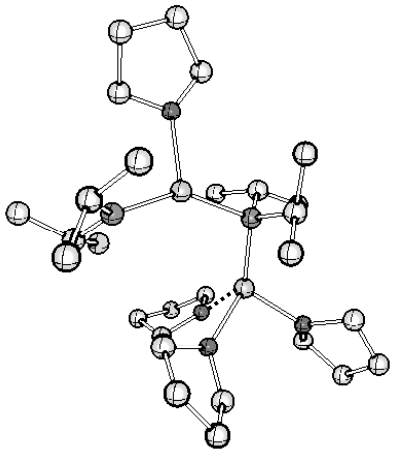
17
G = -1295.461072
G_{MP2} = -1290.892143
ΔG = 14.9 kcal/mol
ΔG_{MP2} = 13.5 kcal/mol
(TS optimization with 6-31+G(d) basis set).

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.045825	-0.614018	-2.831515	H	4.542758	1.915379	0.738981
N	0.252230	-1.234589	-1.528756	C	4.539090	2.143615	-1.389844
Li	-0.929733	-0.635010	-0.044926	H	5.412292	1.517531	-1.608566
O	-2.876562	-1.152434	0.064566	H	3.849123	2.059178	-2.241139
C	-3.978872	-0.222572	0.060737	H	4.882730	3.188135	-1.325407
C	-5.148184	-1.011264	0.662805	C	2.596971	2.549580	0.159017
C	-4.840061	-2.482649	0.266972	H	2.169062	2.345581	1.147545
C	-3.428207	-2.418559	-0.354749	H	2.837960	3.620382	0.104151
H	-3.466252	-2.439721	-1.451383	H	1.823863	2.345675	-0.594777
H	-2.749205	-3.201232	-0.011284	C	4.649542	-0.558437	0.274579
H	-5.564589	-2.876474	-0.452666	H	5.586555	-0.152836	-0.163464
H	-4.859655	-3.137828	1.143260	C	4.510284	-1.984916	-0.277767
H	-6.112829	-0.663794	0.279583	H	3.603667	-2.466816	0.118545
H	-5.163894	-0.898410	1.751988	H	4.442633	-1.973790	-1.373321
H	-3.665151	0.660241	0.619128	H	5.361047	-2.619067	0.005453
H	-4.187923	0.073987	-0.978041	C	4.889644	-0.631962	1.805501
O	-0.482864	-0.286274	1.847942	H	5.825024	-1.157488	2.052888
C	-1.380346	-0.527023	2.949470	H	4.946813	0.371971	2.243641
C	-0.539634	-1.239780	4.032609	H	4.059332	-1.163817	2.291507
C	0.929004	-1.004076	3.583978	H	0.605808	-1.022916	-3.627535
C	0.800690	0.014974	2.449236	C	0.253888	0.891238	-2.767613
H	1.577112	-0.043454	1.678681	H	0.006866	1.386758	-3.715348
H	0.765247	1.043588	2.839224	H	-0.331458	1.372355	-1.971369
H	1.373139	-1.930402	3.206232	H	1.315760	1.085996	-2.569350
H	1.566827	-0.634611	4.392582	C	-1.497513	-0.815766	-3.330923
H	-0.772325	-2.308255	4.079041	H	-1.637460	-0.372185	-4.326471
H	-0.741504	-0.816474	5.022061	H	-1.758803	-1.877592	-3.408730
H	-1.759462	0.440535	3.309674	H	-2.212847	-0.339894	-2.645208
H	-2.216671	-1.113279	2.564836	O	-2.051368	2.489822	0.004120
C	0.200091	-2.705638	-1.569220	C	-1.301101	3.309746	0.922705
H	-0.794376	-3.063873	-1.911204	C	-1.054325	4.633159	0.196465
C	1.228400	-3.373573	-2.512914	C	-2.334790	4.770918	-0.643605
H	1.086904	-3.069732	-3.555730	C	-2.625247	3.314679	-1.032705

Table 1 (continued).

H	2.254268	-3.110258	-2.223059	H	-2.153202	3.047554	-1.987008
H	1.137963	-4.468111	-2.478209	H	-3.697234	3.093894	-1.102039
C	0.392263	-3.273276	-0.151683	H	-2.212016	5.418502	-1.517666
H	-0.360865	-2.893587	0.552658	H	-3.150443	5.178226	-0.033108
H	0.320505	-4.368303	-0.150521	H	-0.172766	4.552275	-0.449913
H	1.377520	-3.004862	0.250681	H	-0.896725	5.468991	0.885925
Li	2.018257	-0.520613	-0.918410	H	-1.895717	3.461761	1.837013
N	3.501941	0.259879	-0.093801	H	-0.384900	2.773307	1.181944
C	3.839086	1.676967	-0.086507				





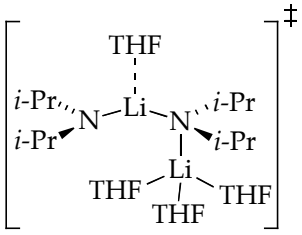
18
G = -1527.803259
G_{MP2} = -1522.470944
ΔG = 19.5 kcal/mol
ΔG_{MP2} = 10.2 kcal/mol
(TS optimization with 6-31+G(d) basis set).

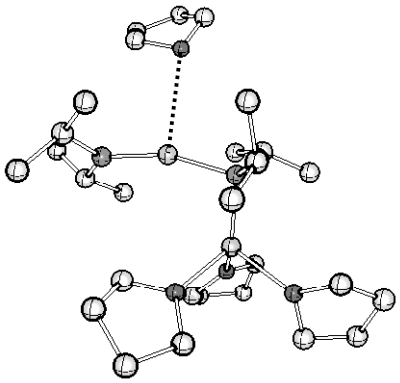
Atom	X	Y	Z	Atom	X	Y	Z
C	-0.196447	-2.460616	0.817736	H	-0.453385	1.605560	1.285197
N	-0.165669	-1.526945	-0.318073	H	-1.018572	2.935312	2.321953
Li	1.468548	-0.365725	-0.292304	H	-1.901133	1.393882	2.284246
O	3.336883	-1.207007	-0.729352	C	-3.443932	1.881708	-1.457309
C	4.478112	-1.217170	0.148589	H	-4.423831	2.232223	-1.057149
C	5.690135	-1.494232	-0.760678	C	-3.769097	0.640237	-2.303469
C	5.070129	-2.173658	-2.014775	H	-2.871864	0.277111	-2.822876
C	3.570806	-2.261563	-1.681747	H	-4.150551	-0.176100	-1.677816
H	3.314927	-3.223900	-1.217672	H	-4.525742	0.863889	-3.067578
H	2.907577	-2.092325	-2.531370	C	-2.964801	3.009175	-2.408430
H	5.495029	-3.163052	-2.211304	H	-3.730961	3.245895	-3.161293
H	5.232528	-1.561404	-2.907563	H	-2.741286	3.935220	-1.864777
H	6.424567	-2.132762	-0.259457	H	-2.052197	2.700404	-2.936979
H	6.196290	-0.562458	-1.032939	O	-3.558047	-1.369285	0.769814
H	4.494834	-0.258024	0.667027	C	-3.936765	-2.726034	1.043099
H	4.345347	-2.017837	0.891433	C	-5.476967	-2.777258	0.904550
O	1.769377	1.441675	-1.044857	C	-5.903455	-1.283544	0.928928
C	2.988911	1.961597	-1.599748	C	-4.611217	-0.548372	1.306437

Table 1 (continued).

C	2.595253	2.600864	-2.948680	H	-4.494165	-0.485595	2.401084
C	1.057673	2.801119	-2.832816	H	-4.478704	0.442828	0.871111
C	0.741892	2.405820	-1.385937	H	-6.711729	-1.085137	1.640742
H	-0.236795	1.937059	-1.231309	H	-6.243572	-0.962270	-0.060955
H	0.840935	3.266467	-0.708144	H	-5.924715	-3.348357	1.725032
H	0.527380	2.143356	-3.528542	H	-5.776070	-3.258706	-0.031955
H	0.747067	3.828335	-3.046437	H	-3.405878	-3.364963	0.336130
H	2.843390	1.940062	-3.785543	H	-3.620442	-2.989392	2.063970
H	3.127897	3.544721	-3.105794	H	-1.075067	-3.133426	0.766816
H	3.398990	2.714272	-0.909305	C	-0.340003	-1.669960	2.127507
H	3.691238	1.130452	-1.679330	H	-0.310491	-2.335707	3.000756
C	-0.195324	-2.211705	-1.620168	H	0.473088	-0.939447	2.228312
H	0.635637	-2.943678	-1.715532	H	-1.286679	-1.119716	2.162428
C	-1.481347	-3.023967	-1.913092	C	1.029777	-3.402289	0.937101
H	-1.631020	-3.824796	-1.179903	H	0.914552	-4.091133	1.785951
H	-2.368113	-2.376440	-1.895938	H	1.164684	-4.014966	0.038001
H	-1.428256	-3.497711	-2.903358	H	1.951282	-2.824468	1.093609
C	0.006113	-1.189761	-2.752509	O	2.687943	0.673635	2.141310
H	0.964814	-0.662154	-2.663485	C	2.598826	2.104309	2.297767
H	-0.013963	-1.677350	-3.736028	C	2.372380	2.341950	3.790337
H	-0.782411	-0.428464	-2.734923	C	3.209736	1.212669	4.413121
Li	-1.878772	-0.286358	-0.119542	C	3.010177	0.064521	3.411986
N	-2.518301	1.533126	-0.389943	H	2.176639	-0.587642	3.698297
C	-2.226424	2.628391	0.516873	H	3.906964	-0.554958	3.288454
H	-1.638447	3.445861	0.027258	H	2.889027	0.941413	5.424025
C	-3.451777	3.351064	1.137397	H	4.266129	1.504962	4.461991
H	-4.079083	3.831038	0.378093	H	1.310899	2.219793	4.035774
H	-4.081380	2.643660	1.695167	H	2.686208	3.340671	4.111522
H	-3.124397	4.136101	1.834378	H	3.541186	2.565117	1.961266
C	-1.346446	2.114993	1.667865	H	1.785505	2.459783	1.661939

Table 1 (continued).



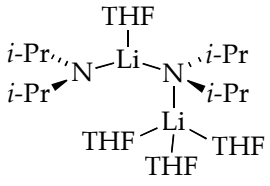


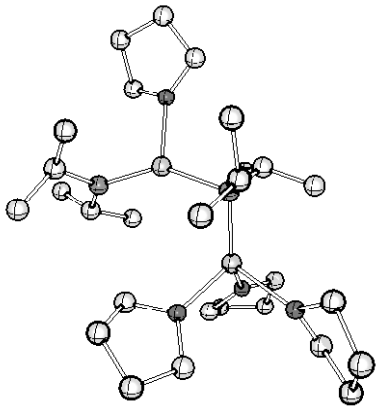
19
G = -1527.803269
G_{MP2} = -1522.469999
ΔG = 19.5 kcal/mol
ΔG_{MP2} = 6.3 kcal/mol
(TS optimization with 6-31+G(d) basis set).

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.238871	-2.426705	-0.404391	C	0.661661	0.119411	-3.057158
N	0.029759	-1.106138	-1.004037	H	1.675673	0.330677	-2.697698
Li	1.662223	-0.150980	-0.189125	H	0.695877	0.080494	-4.153664
O	2.281252	-0.241571	1.878914	H	0.026599	0.968248	-2.772044
C	2.427056	0.939779	2.707827	Li	-1.478394	0.136465	-0.457200
C	2.657552	0.430601	4.133235	N	-2.415818	1.679612	0.112992
C	3.349155	-0.920147	3.888973	C	-2.357183	2.198724	1.468824
C	2.619905	-1.423663	2.642810	H	-1.827045	3.182221	1.520191
H	1.695603	-1.953458	2.902686	C	-3.723584	2.440657	2.158807
H	3.225625	-2.074455	2.005090	H	-4.325728	3.192824	1.636805
H	3.258657	-1.613000	4.731629	H	-4.304752	1.508585	2.192439
H	4.417335	-0.774681	3.682783	H	-3.581640	2.793815	3.190372
H	1.700054	0.282109	4.646256	C	-1.545100	1.237535	2.350261
H	3.258205	1.124569	4.729891	H	-0.566257	1.023138	1.901987
H	3.284638	1.516255	2.336140	H	-1.375873	1.655151	3.352663
H	1.525195	1.546046	2.603596	H	-2.072908	0.281515	2.464347
O	3.589118	-0.767341	-0.878866	C	-3.260134	2.455913	-0.783573
C	4.855662	-0.559871	-0.237070	H	-4.315258	2.484481	-0.429836
C	5.609444	-1.897433	-0.371172	C	-3.303492	1.789215	-2.165959
C	4.926582	-2.585088	-1.587918	H	-2.306369	1.793115	-2.629282
C	3.874539	-1.560238	-2.045770	H	-3.641468	0.748230	-2.090421
H	2.935224	-1.995474	-2.384775	H	-3.986127	2.315624	-2.846249
H	4.271807	-0.902817	-2.834398	C	-2.845464	3.938857	-0.965176
H	4.444369	-3.519118	-1.284621	H	-3.550636	4.468415	-1.622192
H	5.634078	-2.820073	-2.389429	H	-2.818946	4.477255	-0.010197
H	5.493472	-2.503752	0.532753	H	-1.845639	4.004800	-1.416419
H	6.681427	-1.737233	-0.525176	H	-1.026417	-2.962526	-0.965046
H	5.393651	0.249558	-0.754566	C	-0.783382	-2.264863	1.023323
H	4.652765	-0.250814	0.789370	H	-0.876710	-3.235583	1.529220
O	1.928296	1.898520	-0.333113	H	-0.121387	-1.630484	1.625645
C	3.089354	2.494365	-0.957756	H	-1.780236	-1.807841	1.017712
C	2.739373	3.968629	-1.231038	C	0.981701	-3.381552	-0.390295
C	1.202781	3.978952	-1.163534	H	0.711160	-4.370295	0.007641

Table 1 (continued).

C	0.927207	2.925640	-0.097381	H	1.379400	-3.537467	-1.400307
H	-0.064673	2.461753	-0.157825	H	1.791900	-2.976852	0.231016
H	1.075043	3.338412	0.911922	O	-4.160373	-1.936187	-0.413705
H	0.765667	3.669955	-2.120257	C	-5.142472	-0.960933	-0.047118
H	0.790739	4.958113	-0.901058	C	-5.890000	-1.575565	1.151294
H	3.132297	4.311735	-2.193642	C	-5.714114	-3.107199	0.944563
H	3.157813	4.615290	-0.450291	C	-4.808336	-3.201647	-0.305159
H	3.950351	2.384344	-0.286825	H	-5.408471	-3.389831	-1.211482
H	3.293243	1.936163	-1.877876	H	-4.030634	-3.967729	-0.237438
C	0.110138	-1.191124	-2.473028	H	-6.668732	-3.621064	0.787014
H	0.813396	-1.992553	-2.788561	H	-5.232244	-3.566764	1.813856
C	-1.226745	-1.519379	-3.184535	H	-6.941805	-1.270951	1.176029
H	-1.680814	-2.441624	-2.808195	H	-5.430176	-1.255766	2.092249
H	-1.955583	-0.711866	-3.043030	H	-4.607962	-0.033469	0.171733
H	-1.073029	-1.645734	-4.265981	H	-5.828549	-0.794962	-0.895112





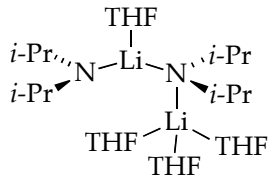
20a
G = -1527.804376
G_{MP2} = -1522.476652
ΔG = 18.8 kcal/mol
ΔG_{MP2} = 4.4 kcal/mol
(connects to **18**)

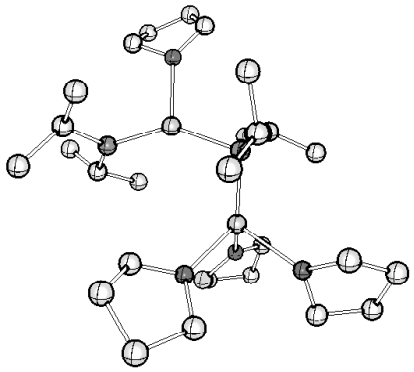
Atom	X	Y	Z	Atom	X	Y	Z
C	-0.220100	-2.602555	0.340672	H	-0.596782	1.199732	1.751442
N	-0.130639	-1.400117	-0.501945	H	-1.197381	2.263832	3.046307
Li	1.521602	-0.284739	-0.002248	H	-2.097546	0.800028	2.597454
O	3.436514	-0.981493	-0.801971	C	-3.399405	2.178875	-1.006747
C	4.689411	-0.975323	-0.106090	H	-4.397238	2.442808	-0.589969
C	5.770488	-0.920519	-1.202703	C	-3.681355	1.172838	-2.133241
C	5.047078	-1.482596	-2.458187	H	-2.757156	0.925542	-2.672979
C	3.640187	-1.833196	-1.942514	H	-4.094937	0.240378	-1.731404
H	3.580319	-2.883135	-1.623317	H	-4.393328	1.576062	-2.865260
H	2.835443	-1.635002	-2.649914	C	-2.866037	3.488110	-1.641733
H	5.550407	-2.358348	-2.878089	H	-3.596547	3.923502	-2.338190
H	4.992811	-0.724635	-3.245442	H	-2.644203	4.246953	-0.882177
H	6.650053	-1.508959	-0.925027	H	-1.941045	3.292745	-2.200724
H	6.103223	0.107959	-1.372199	O	-3.584953	-1.516354	0.316089

Table 1 (continued).

H	4.685692	-0.120925	0.572108	C	-4.003830	-2.876855	0.160444
H	4.780691	-1.898831	0.485592	C	-5.530059	-2.823928	-0.083011
O	1.787724	1.688006	-0.513791	C	-5.931719	-1.399486	0.389952
C	3.007604	2.273195	-1.002630	C	-4.645900	-0.857729	1.028143
C	2.602554	3.397118	-1.988348	H	-4.589326	-1.129968	2.094887
C	1.057732	3.365997	-1.969539	H	-4.465345	0.211734	0.912565
C	0.746275	2.685273	-0.640170	H	-6.768263	-1.407359	1.095602
H	-0.225268	2.178710	-0.594074	H	-6.219763	-0.777627	-0.463150
H	0.827386	3.394770	0.197351	H	-6.045095	-3.609734	0.478768
H	0.670917	2.757234	-2.793230	H	-5.767512	-2.967790	-1.141288
H	0.610788	4.361134	-2.045063	H	-3.435851	-3.305239	-0.666098
H	3.006173	3.226928	-2.990988	H	-3.769842	-3.437912	1.077924
H	2.981825	4.364424	-1.642679	H	-1.030088	-3.277291	0.001573
H	3.583129	2.676333	-0.156504	C	-0.586256	-2.204226	1.779231
H	3.582896	1.468354	-1.463417	H	-0.544868	-3.066135	2.458681
C	-0.073830	-1.730097	-1.934660	H	0.101338	-1.437512	2.153890
H	0.760203	-2.428673	-2.161118	H	-1.599251	-1.791425	1.826088
C	-1.335283	-2.421592	-2.509301	C	1.056822	-3.480130	0.358224
H	-1.534753	-3.379771	-2.017619	H	0.913426	-4.381846	0.969590
H	-2.222279	-1.786164	-2.387101	H	1.331218	-3.810275	-0.650088
H	-1.214992	-2.628837	-3.581306	H	1.910394	-2.924104	0.769903
C	0.196716	-0.459699	-2.755988	O	2.338128	-0.007549	1.994469
H	1.143482	0.013480	-2.470949	C	2.387995	1.320192	2.572907
H	0.236709	-0.680734	-3.830468	C	2.551761	1.110427	4.077657
H	-0.594140	0.282051	-2.592212	C	3.379154	-0.182078	4.127543
Li	-1.869401	-0.248064	-0.150765	C	2.780414	-0.982841	2.969244
N	-2.534703	1.577768	-0.003848	H	1.916095	-1.573208	3.291945
C	-2.302323	2.421160	1.154060	H	3.496103	-1.653691	2.485508
H	-1.682013	3.321332	0.916866	H	3.303525	-0.712736	5.081241
C	-3.564567	2.994359	1.849184	H	4.438469	0.034937	3.943083
H	-4.148150	3.636649	1.180921	H	1.573952	0.958413	4.548760
H	-4.223494	2.184886	2.191807	H	3.038686	1.959114	4.567348
H	-3.288461	3.598940	2.724188	H	3.246337	1.857860	2.147980
C	-1.499925	1.631611	2.199937	H	1.473106	1.847178	2.299874

Table 1 (continued).



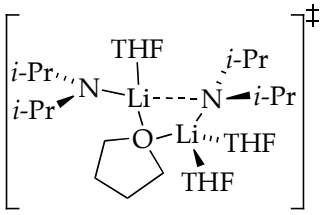


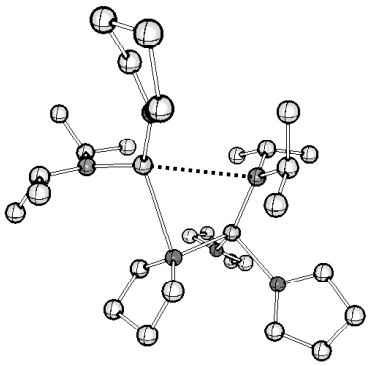
20b
G = -1527.803906
G_{MP2} = -1522.478074
ΔG = 19.1 kcal/mol
ΔG_{MP2} = 3.5 kcal/mol
(connects to **19** and **21**)

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.084948	-2.606720	-0.058656	O	1.688377	1.888125	-0.547285
N	-0.055665	-1.326339	-0.780619	Li	-1.852230	-0.278723	-0.326158
Li	1.494492	-0.122263	-0.150949	N	-2.538252	1.499965	0.081021
O	2.219285	0.095245	1.882731	C	-2.404870	2.124972	1.384549
C	2.302024	1.404017	2.499872	H	-1.873793	3.107194	1.335315
C	2.540024	1.148167	3.988503	C	-3.728245	2.427781	2.132955
C	3.333920	-0.165765	3.965086	H	-4.380850	3.098396	1.563736
C	2.655995	-0.917874	2.818514	H	-4.285807	1.499822	2.321108
H	1.782249	-1.479556	3.167710	H	-3.532105	2.905758	3.102860
H	3.320519	-1.608174	2.289927	C	-1.541977	1.233855	2.289538
H	3.291023	-0.718856	4.908019	H	-0.598780	0.973644	1.794673
H	4.388615	0.027460	3.732831	H	-1.309056	1.726205	3.243999
H	1.584930	1.008007	4.507419	H	-2.064213	0.294034	2.515254
H	3.073645	1.971175	4.473338	C	-3.426777	2.210448	-0.826199
H	3.136690	1.952393	2.044127	H	-4.477668	2.231927	-0.453049
H	1.375502	1.941127	2.293494	C	-3.485710	1.480496	-2.176919
C	-0.002232	-1.533121	-2.236810	H	-2.502609	1.500602	-2.666203
H	0.790458	-2.262417	-2.512403	H	-3.776185	0.430999	-2.048620
C	-1.299116	-2.095685	-2.869954	H	-4.208216	1.949104	-2.857906
H	-1.610533	-3.031477	-2.395182	C	-3.068886	3.694087	-1.095547
H	-2.125597	-1.380511	-2.774786	H	-3.820823	4.170217	-1.740052
H	-1.156293	-2.303396	-3.939455	H	-3.011854	4.279113	-0.170650
C	0.354535	-0.221026	-2.952399	H	-2.097174	3.770524	-1.600476
H	1.344766	0.145974	-2.659175	O	-3.597800	-1.608569	-0.217104
H	0.352981	-0.348765	-4.042500	C	-4.825404	-0.981956	0.193266
H	-0.372777	0.561051	-2.702830	C	-5.359492	-1.901708	1.293337
H	-0.804371	-3.311841	-0.520002	C	-4.919665	-3.309770	0.815529
C	-0.566415	-2.391519	1.384710	C	-3.874004	-3.014220	-0.289891
H	-0.499149	-3.314641	1.975761	H	-4.272215	-3.255329	-1.285944
H	0.037549	-1.623362	1.880757	H	-2.928429	-3.541870	-0.156121
H	-1.608142	-2.053442	1.409244	H	-5.760404	-3.881999	0.410149
C	1.262313	-3.373320	-0.036976	H	-4.489755	-3.895554	1.633618
H	1.162982	-4.344729	0.467309	H	-6.442621	-1.814888	1.423912

Table 1 (continued).

H	1.627051	-3.571637	-1.051301	H	-4.883666	-1.652385	2.247727
H	2.033525	-2.795376	0.488848	H	-4.560734	0.029196	0.502302
O	3.472215	-0.647330	-0.871708	H	-5.519515	-0.941619	-0.661374
C	4.729895	-0.358088	-0.249191	C	2.815575	2.465746	-1.240705
C	5.544863	-1.661585	-0.348655	C	2.345489	3.820158	-1.803044
C	4.898785	-2.405326	-1.551024	C	0.813292	3.702133	-1.753136
C	3.792218	-1.445475	-2.022297	C	0.604882	2.854463	-0.504359
H	2.876032	-1.936371	-2.348171	H	-0.345607	2.305932	-0.463780
H	4.153070	-0.787648	-2.828105	H	0.709548	3.466500	0.404310
H	4.467046	-3.356881	-1.228986	H	0.433270	3.171851	-2.633701
H	5.615372	-2.616835	-2.350177	H	0.309938	4.671141	-1.693252
H	5.448271	-2.251668	0.567633	H	2.734022	4.004727	-2.809279
H	6.609231	-1.458064	-0.499892	H	2.682900	4.641278	-1.160045
H	5.227481	0.458654	-0.794773	H	3.655015	2.574158	-0.542094
H	4.519466	-0.026570	0.767778	H	3.113411	1.766516	-2.028012





21
G = -1527.783839
G_{MP2} = -1522.449067
ΔG = 31.6 kcal/mol
ΔG_{MP2} = 21.7 kcal/mol

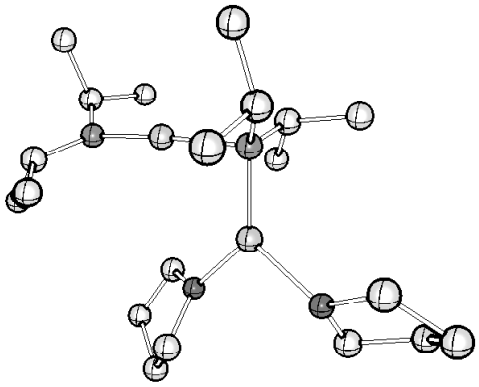
Atom	X	Y	Z	Atom	X	Y	Z
C	1.103940	1.633539	-2.616314	O	0.285328	-0.703361	1.443430
N	0.919494	1.595045	-1.169017	Li	-2.051919	0.044382	-0.074471
Li	1.593178	0.139784	-0.059698	N	-3.067364	-1.558909	-0.137854
O	2.591887	-1.734877	-0.741140	C	-3.117930	-2.414348	-1.312427
C	2.028028	-2.839289	-1.491943	H	-2.883101	-3.475298	-1.071623
C	3.081312	-3.221845	-2.530858	C	-4.482866	-2.452302	-2.043657
C	4.386135	-2.898612	-1.789115	H	-5.286829	-2.811173	-1.391854
C	4.007388	-1.630408	-1.020075	H	-4.759173	-1.446736	-2.390465
H	4.176277	-0.729191	-1.622445	H	-4.448838	-3.117067	-2.917800
H	4.540292	-1.521554	-0.072089	C	-2.043525	-1.967055	-2.309248
H	5.238884	-2.740712	-2.456271	H	-1.058355	-1.960581	-1.827574
H	4.642692	-3.708223	-1.095260	H	-1.990693	-2.624849	-3.186207
H	2.981982	-2.593592	-3.422820	H	-2.247016	-0.948555	-2.671527

Table 1 (continued).

H	3.002504	-4.268854	-2.838298	C	-4.023378	-1.931099	0.893268
H	1.828848	-3.670094	-0.801792	H	-5.073424	-1.877988	0.528505
H	1.083029	-2.508775	-1.926504	C	-3.951153	-0.936535	2.061602
C	0.772759	2.928671	-0.605012	H	-2.951591	-0.950875	2.520682
H	1.689249	3.553763	-0.746686	H	-4.147573	0.083584	1.713534
C	-0.375486	3.785387	-1.198553	H	-4.680811	-1.175798	2.845602
H	-0.210499	4.020057	-2.255200	C	-3.864453	-3.366983	1.453608
H	-1.324817	3.242291	-1.120455	H	-4.624120	-3.583325	2.217459
H	-0.467450	4.743564	-0.667598	H	-3.966159	-4.124340	0.668646
C	0.581380	2.842668	0.916230	H	-2.873757	-3.496662	1.909316
H	1.431730	2.341198	1.392293	O	-3.065517	1.772657	0.002608
H	0.482074	3.837903	1.369608	C	-3.290067	2.805188	0.990135
H	-0.320801	2.265403	1.154316	C	-4.470510	3.630967	0.471097
H	0.286077	2.188725	-3.118792	C	-5.262989	2.593713	-0.339721
C	1.058797	0.221878	-3.208770	C	-4.146450	1.763388	-0.969540
H	1.133206	0.243515	-4.303813	H	-3.778265	2.219066	-1.897809
H	1.893809	-0.379501	-2.828211	H	-4.400377	0.715384	-1.147751
H	0.124645	-0.278967	-2.937442	H	-5.921291	3.042519	-1.089593
C	2.415669	2.316870	-3.082289	H	-5.874089	1.971538	0.324496
H	2.488562	2.347627	-4.178553	H	-4.113184	4.434798	-0.182813
H	2.491169	3.349339	-2.722350	H	-5.048422	4.083304	1.282822
H	3.287144	1.766765	-2.698542	H	-3.525576	2.322415	1.947585
O	3.349495	0.684193	1.032764	H	-2.369793	3.383072	1.099004
C	3.959380	0.209072	2.250534	C	0.249967	-0.183018	2.790691
C	5.293130	0.953587	2.382638	C	0.595316	-1.364292	3.693201
C	5.003107	2.265282	1.637032	C	-0.097747	-2.523215	2.961149
C	4.123063	1.781699	0.486145	C	0.077098	-2.152394	1.482989
H	4.729840	1.405682	-0.348356	H	-0.808157	-2.371408	0.875649
H	3.421946	2.521528	0.100015	H	0.969895	-2.613303	1.052593
H	5.906696	2.773855	1.287984	H	-1.160124	-2.555665	3.224274
H	4.447698	2.958820	2.279562	H	0.335435	-3.500816	3.194064
H	6.094857	0.399940	1.879417	H	0.241465	-1.224482	4.719593
H	5.587457	1.098058	3.426485	H	1.681098	-1.517175	3.722553
H	3.290385	0.437760	3.089910	H	0.952726	0.649902	2.847488
H	4.073201	-0.878747	2.187124	H	-0.758314	0.195485	3.008439

Table 2. Optimized geometries of THF disolvated LDA open dimers at the B3LYP level of theory with a 6-31G(d) basis set at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z). Single point MP2 energies are included. A representative image is shown in Table 2a. The geometries of the open dimers are categorized most conveniently by two pseudo-dihedral angles ω_C and ω_O as shown in Table 2b. ω_C is defined by a dihedral angle spanning atoms C-N-N-C and ω_O is defined by a dihedral angle spanning atoms O-Li-N-Li. Although the direction of the arrow is irrelevant for the measure of the dihedral angle, it indicates the sign of the angle (clockwise = minus , counter-clockwise = plus). The caption below the energy values indicates the connectivity of transition states and ground states. Structure **4i** and **4j** represent the meso stereoisomer in contrast to the homochiral form.

a)



b)

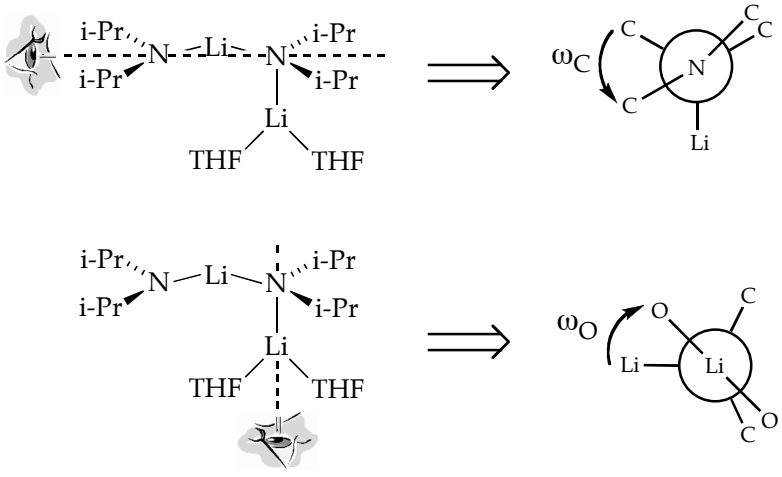
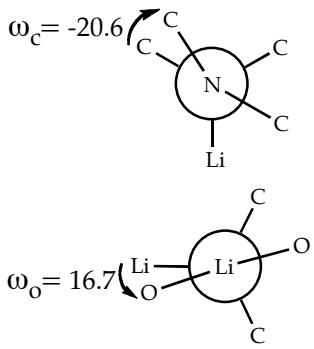
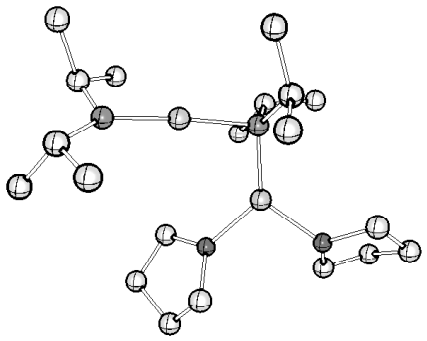


Table 2 (continued).



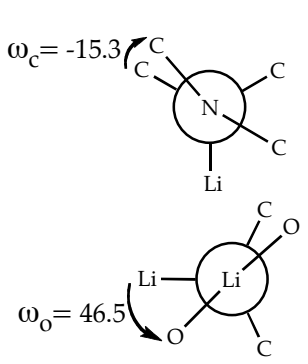


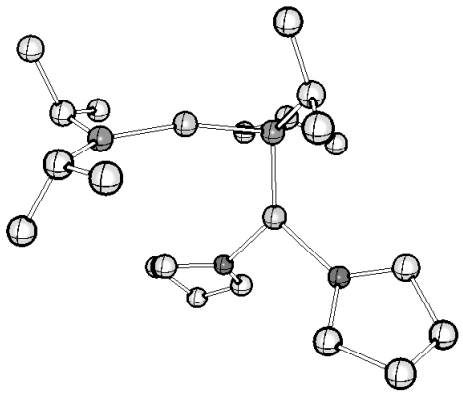
4a
G = -1063.121401
G_{MP2} = 1059.32551
ΔG = 8.8 kcal/mol
ΔG_{MP2} = 11.5 kcal/mol
4a → 11

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.562689	-2.265881	-1.273584	H	4.429804	-2.626589	0.038385
N	-0.399930	-1.595055	0.026309	H	5.865412	-2.071460	-0.860057
Li	-1.310697	0.120142	0.137474	C	3.541530	-1.160201	-2.099251
O	-3.235353	0.436506	0.443202	H	3.007426	-0.359350	-2.624624
C	-4.029225	1.203369	-0.492261	H	4.283446	-1.588171	-2.785653
C	-5.252234	0.337764	-0.784390	H	2.818445	-1.958504	-1.868778
C	-5.491255	-0.335016	0.576788	C	3.716840	0.761867	1.113708
C	-4.065631	-0.570460	1.089302	H	4.616486	0.320037	1.592664
H	-3.676453	-1.552632	0.804545	C	2.693137	0.953929	2.242040
H	-3.969694	-0.450763	2.172290	H	1.750785	1.353316	1.835476
H	-6.060372	-1.265821	0.502436	H	2.472772	-0.002082	2.732897
H	-6.035840	0.341466	1.245451	H	3.048490	1.655288	3.008069
H	-5.013673	-0.411132	-1.548190	C	4.164044	2.153674	0.598371
H	-6.106823	0.924543	-1.133515	H	4.655911	2.742686	1.385944
H	-4.312377	2.156872	-0.026069	H	4.869370	2.063067	-0.234927
H	-3.407765	1.411239	-1.367486	H	3.297195	2.722807	0.236351
O	-0.603464	1.905058	-0.151897	C	-0.574569	-2.487002	1.182124
C	-0.887718	3.024742	0.712892	H	-1.566770	-2.981261	1.165061
C	-0.618184	4.254224	-0.148305	C	0.466186	-3.625332	1.276162
C	0.617291	3.806938	-0.948377	H	0.448645	-4.264177	0.386312
C	0.392800	2.299835	-1.150099	H	1.483281	-3.219260	1.373752
H	1.299551	1.703356	-0.994149	H	0.276594	-4.267165	2.146480
H	-0.034153	2.068828	-2.131333	C	-0.536210	-1.659692	2.476371
H	1.528283	3.979679	-0.366358	H	-1.317795	-0.885770	2.483629
H	0.723834	4.335881	-1.899723	H	-0.694106	-2.290369	3.359538
H	-0.441733	5.154365	0.448084	H	0.431381	-1.155963	2.598075
H	-1.468903	4.443972	-0.813861	H	0.236789	-3.015070	-1.451066
H	-1.921894	2.924299	1.052963	C	-0.428671	-1.226974	-2.397830
H	-0.220070	2.991558	1.584643	H	-0.461499	-1.699860	-3.386492
Li	1.486537	-0.889513	0.111808	H	-1.254526	-0.498132	-2.358481
N	3.172123	-0.107185	0.086603	H	0.514166	-0.673167	-2.325483
C	4.190495	-0.630117	-0.812129	C	-1.894589	-3.025529	-1.460779

Table 2 (continued).

H	4.899759	0.161283	-1.133400	H	-1.956928	-3.462767	-2.465456
C	5.055888	-1.752377	-0.187374	H	-2.012275	-3.843485	-0.742401
H	5.517601	-1.424477	0.750723	H	-2.747525	-2.342387	-1.335210



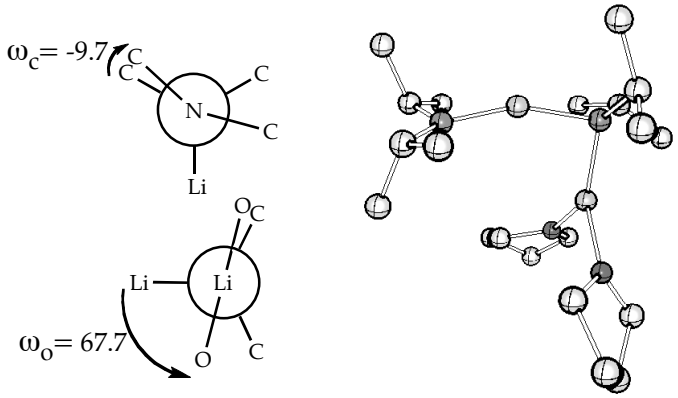


4b
G = -1063.120567
G_{MP2} = -1059.324222
ΔG = 9.4 kcal/mol
ΔG_{MP2} = 12.3 kcal/mol
10* → 4b

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.052490	0.079073	-2.158608	H	2.480688	-2.296775	2.332048
N	-2.945568	-0.124926	-0.720981	C	-0.467076	-0.570685	2.989759
Li	-1.543941	-1.024750	0.143024	H	-1.536162	-0.712774	2.800384
N	0.251114	-1.606019	0.853742	H	-0.320001	-0.557325	4.077030
Li	1.235801	-0.018706	0.231005	H	-0.193171	0.420631	2.602895
O	0.746132	1.874179	0.396741	H	-0.010142	-2.630984	2.706565
C	1.465056	2.741014	1.310151	C	0.602097	-2.901437	0.243918
C	0.579732	3.979316	1.519237	C	-0.525862	-3.954211	0.350965
C	-0.820583	3.464856	1.146782	H	-1.401156	-3.645811	-0.238879
C	-0.511370	2.501696	0.008121	H	-0.203484	-4.936334	-0.021137
H	-0.352900	3.039937	-0.936650	H	-0.852687	-4.085587	1.388644
H	-1.258434	1.712654	-0.146766	C	0.985729	-2.726549	-1.232741
H	-1.504770	4.262418	0.843482	H	1.846204	-2.054726	-1.344385
H	-1.274645	2.924216	1.985142	H	1.246700	-3.686816	-1.694665
H	0.881149	4.784619	0.839599	H	0.153716	-2.301596	-1.806981
H	0.644888	4.361643	2.542135	H	1.485886	-3.342484	0.745710
H	1.622399	2.187715	2.243586	C	-4.211554	0.114840	-0.041276
H	2.442809	2.980993	0.878117	C	-3.992554	0.291960	1.467274
O	3.060112	0.161525	-0.492913	H	-3.292671	1.111561	1.671056
C	4.209960	-0.672552	-0.196333	H	-4.932675	0.502023	1.993042
C	5.348351	-0.117265	-1.052956	H	-3.577986	-0.627920	1.906788
C	4.595854	0.409884	-2.284547	C	-5.262910	-1.002688	-0.256006
C	3.321536	0.980604	-1.660701	H	-4.910551	-1.941016	0.193988
H	2.449117	0.929572	-2.318409	H	-6.231398	-0.745580	0.197185
H	3.456106	2.019450	-1.335358	H	-5.438147	-1.191223	-1.320794
H	4.351985	-0.413525	-2.965457	H	-4.688975	1.054739	-0.391114

Table 2 (continued).

H	5.155782	1.162553	-2.846951	C	-1.874966	-0.581017	-2.886707
H	6.094418	-0.879276	-1.295504	H	-1.871606	-1.664476	-2.716602
H	5.856113	0.703808	-0.533334	H	-1.910229	-0.405705	-3.969723
H	4.396996	-0.620543	0.879055	H	-0.920311	-0.173223	-2.518753
H	3.965428	-1.707566	-0.462237	C	-3.135448	1.566455	-2.590858
C	0.372303	-1.667534	2.321564	H	-2.185214	2.081009	-2.395670
C	1.834522	-1.559252	2.821673	H	-3.355834	1.664062	-3.663593
H	2.243499	-0.558275	2.610279	H	-3.922070	2.098321	-2.044152
H	1.910107	-1.720007	3.905767	H	-3.965078	-0.400070	-2.569689

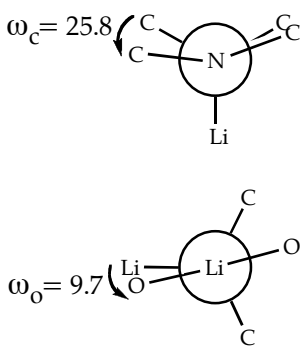


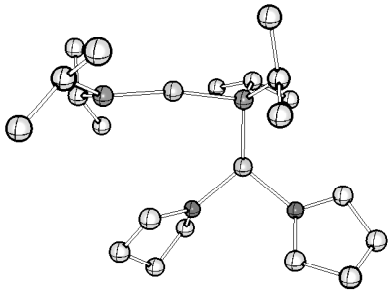
4c
G = -1063.117200
G_{MP2} = -1059.321171
ΔG = 11.5 kcal/mol
ΔG_{MP2} = 14.2 kcal/mol
10 → 4c

Atom	X	Y	Z	Atom	X	Y	Z
C	2.312152	-0.161294	-2.482859	H	-1.900783	2.835830	-0.424085
N	2.515584	-0.208852	-1.041866	C	1.187960	4.004118	0.664634
Li	1.635958	0.949284	0.145295	H	1.785507	3.928480	1.580629
N	0.112899	1.786433	1.172560	H	0.995469	5.070093	0.479790
Li	-1.117424	0.373718	0.532673	H	1.800655	3.627229	-0.167216
O	-2.653178	0.295854	-0.732762	H	-0.732427	3.698528	1.556720
C	-3.926632	-0.238159	-0.298309	C	0.274847	1.700904	2.636886
C	-4.648684	-0.682271	-1.572127	C	1.193659	0.538959	3.036660
C	-4.095205	0.301761	-2.614177	H	0.854046	-0.403284	2.588639
C	-2.638050	0.444745	-2.176175	H	1.227577	0.402467	4.125206
H	-2.005201	-0.343419	-2.602072	H	2.221219	0.716450	2.696566
H	-2.197519	1.415981	-2.409752	C	-1.076840	1.589816	3.381838
H	-4.185854	-0.060114	-3.642283	H	-1.754520	2.396813	3.079173
H	-4.612436	1.265678	-2.544225	H	-0.957535	1.644442	4.473106
H	-4.370717	-1.710401	-1.831954	H	-1.570635	0.633016	3.152913
H	-5.736806	-0.639920	-1.468954	H	0.757464	2.617844	3.021652
H	-4.476274	0.555603	0.223627	C	3.732940	-0.934788	-0.701255
H	-3.731315	-1.055580	0.401508	C	5.027491	-0.119463	-0.945020
O	-1.039289	-1.556339	1.032475	H	5.068598	0.266478	-1.969588

Table 2 (continued).

C	-1.444373	-2.273759	2.222769	H	5.932108	-0.723462	-0.781906
C	-1.112099	-3.744469	1.958454	H	5.062259	0.742450	-0.264335
C	0.093068	-3.638492	1.011276	C	3.713012	-1.394168	0.762509
C	-0.277842	-2.435135	0.148796	H	3.643509	-0.530515	1.438569
H	0.579191	-1.868331	-0.235813	H	4.626805	-1.940974	1.028070
H	-0.928124	-2.727251	-0.686963	H	2.853107	-2.044872	0.960440
H	1.010173	-3.433665	1.575008	H	3.833551	-1.858466	-1.310023
H	0.255142	-4.540990	0.414949	C	1.729564	-1.468510	-3.078741
H	-0.894450	-4.290114	2.881371	H	2.320434	-2.339724	-2.773866
H	-1.949584	-4.244784	1.457771	H	1.712249	-1.447689	-4.178265
H	-2.511033	-2.091526	2.393234	H	0.699489	-1.623535	-2.727221
H	-0.881914	-1.878277	3.076262	C	1.397751	1.008767	-2.866172
C	-0.121170	3.191209	0.785983	H	0.425980	0.910166	-2.359730
C	-0.913459	3.302786	-0.522786	H	1.201814	1.044818	-3.945846
H	-0.379797	2.809994	-1.345394	H	1.840824	1.966155	-2.565450
H	-1.061018	4.351405	-0.810250	H	3.266975	0.013440	-3.019569



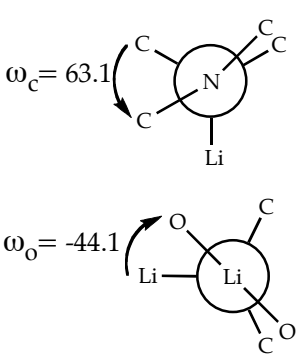


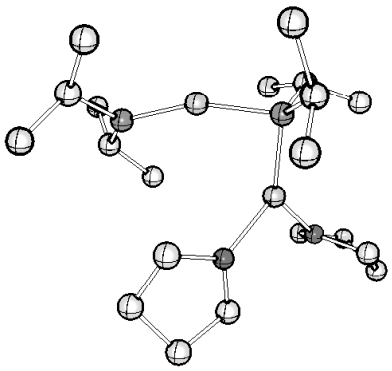
4d
G = -1063.119115
G_{MP2} = -1059.323269
ΔG = 10.3 kcal/mol
ΔG_{MP2} = 12.9 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.746713	-0.163010	-1.560314	H	2.620118	-3.018853	1.441428
N	-3.055397	-0.105518	-0.278875	C	-0.427054	-1.847975	2.638457
Li	-1.467832	-1.067975	0.023677	H	-1.483278	-1.908333	2.347104
N	0.401932	-1.772920	0.312692	H	-0.330151	-2.334846	3.616547
Li	1.292315	-0.014437	0.310747	H	-0.176278	-0.785324	2.772456
O	0.525152	1.769805	0.346420	H	0.135943	-3.540163	1.478991
C	0.694816	2.698195	1.436838	C	0.890564	-2.585542	-0.813480
C	0.357206	4.061651	0.840733	C	-0.059042	-3.732837	-1.227449
C	-0.807812	3.709701	-0.100265	H	-1.006998	-3.332891	-1.609487
C	-0.457220	2.302019	-0.604817	H	0.385228	-4.356459	-2.015083
H	0.033635	2.322417	-1.585075	H	-0.290732	-4.388947	-0.381680
H	-1.321944	1.624122	-0.627675	C	1.153128	-1.688083	-2.034550
H	-0.923184	4.423250	-0.921108	H	1.936214	-0.944128	-1.830158

Table 2 (continued).

H	-1.750455	3.685725	0.456362	H	1.479560	-2.273192	-2.902742
H	1.213381	4.450482	0.276268	H	0.241590	-1.149367	-2.325661
H	0.087635	4.797722	1.604081	H	1.860006	-3.065397	-0.566875
H	0.006248	2.436207	2.251115	C	-3.962714	0.301903	0.787274
H	1.724390	2.605056	1.796192	C	-3.210010	0.985134	1.939757
O	3.225110	0.406603	0.126052	H	-2.719531	1.902616	1.593691
C	4.279895	-0.596033	0.139272	H	-3.883765	1.248208	2.765917
C	5.512152	0.079163	-0.472973	H	-2.435106	0.322291	2.347365
C	4.889744	1.156952	-1.373895	C	-4.800485	-0.872609	1.350784
C	3.693871	1.604686	-0.537877	H	-4.144842	-1.597266	1.853773
H	2.862263	2.010886	-1.117558	H	-5.559335	-0.538184	2.074152
H	3.989242	2.342165	0.220726	H	-5.318547	-1.401410	0.542649
H	4.550313	0.720463	-2.320350	H	-4.696061	1.049576	0.421441
H	5.573441	1.979984	-1.601288	C	-3.010632	-1.084644	-2.541637
H	6.141815	-0.629400	-1.018374	H	-2.962928	-2.109185	-2.151797
H	6.124995	0.543989	0.307934	H	-3.500133	-1.116660	-3.523616
H	4.429821	-0.924913	1.170323	H	-1.981396	-0.730201	-2.703501
H	3.936518	-1.449091	-0.455213	C	-3.941854	1.224071	-2.224768
C	0.487874	-2.498141	1.592189	H	-2.971580	1.647226	-2.519840
C	1.920081	-2.591517	2.168203	H	-4.571720	1.164843	-3.124452
H	2.288223	-1.593202	2.449235	H	-4.417830	1.929223	-1.533621
H	1.954654	-3.221795	3.067013	H	-4.765496	-0.590721	-1.448275





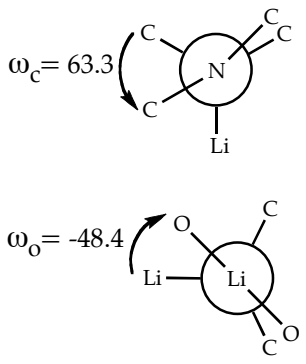
4e
G = -1063.119655
G_{MP2} = -1059.324365
ΔG = 9.9 kcal/mol
ΔG_{MP2} = 12.2 kcal/mol

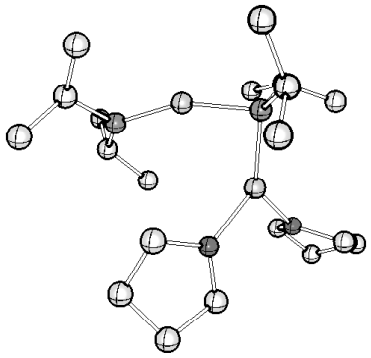
Atom	X	Y	Z	Atom	X	Y	Z
C	-2.736853	0.672998	2.001700	H	2.699703	-3.290804	-0.747489
N	-2.802689	-0.114503	0.781804	C	0.488986	-2.563597	1.835718
Li	-1.462388	-1.241467	0.136308	H	-0.597666	-2.527788	1.989104
N	0.328772	-1.864973	-0.535642	H	0.894099	-3.311227	2.528734
Li	1.102309	-0.040092	-0.436232	H	0.896129	-1.585898	2.130607
O	0.425706	1.732392	-0.963894	H	0.399134	-3.876387	0.165656
C	-0.948053	2.033114	-1.364257	C	0.276527	-2.373699	-1.918641

Table 2 (continued).

C	-1.119561	3.523792	-1.089621	C	-0.896327	-3.345079	-2.185476
C	0.284926	4.070938	-1.385128	H	-1.859543	-2.822746	-2.112420
C	1.186819	2.957396	-0.845334	H	-0.833646	-3.787952	-3.188853
H	1.429125	3.113615	0.213115	H	-0.906863	-4.169306	-1.463597
H	2.121058	2.846899	-1.404948	C	0.200682	-1.213778	-2.921971
H	0.489469	5.034436	-0.908211	H	1.089980	-0.569149	-2.866709
H	0.428291	4.190188	-2.465594	H	0.127308	-1.579222	-3.953417
H	-1.387934	3.688630	-0.039836	H	-0.681238	-0.589031	-2.729285
H	-1.897836	3.972312	-1.713619	H	1.199560	-2.933372	-2.163815
H	-1.047430	1.809135	-2.434080	C	-4.150539	-0.198882	0.237229
H	-1.614671	1.386081	-0.779463	C	-4.249468	-1.368636	-0.752261
O	2.914101	0.484991	0.215997	H	-4.012031	-2.319245	-0.256749
C	3.241011	0.781669	1.595618	H	-5.251925	-1.454453	-1.190532
C	4.718256	0.421262	1.751078	H	-3.543457	-1.227366	-1.585121
C	5.273285	0.738216	0.353269	C	-4.631419	1.094934	-0.467453
C	4.125304	0.297755	-0.558565	H	-4.038899	1.281441	-1.373834
H	4.200013	-0.761998	-0.827837	H	-5.688262	1.029806	-0.763108
H	4.041923	0.892088	-1.473972	H	-4.527240	1.967380	0.187972
H	6.204776	0.211062	0.128404	H	-4.900013	-0.407363	1.028135
H	5.457778	1.813802	0.249324	C	-1.280115	1.040903	2.328259
H	4.829047	-0.645574	1.975249	H	-0.816751	1.592640	1.501431
H	5.203574	0.990865	2.548738	H	-1.211155	1.655853	3.235120
H	3.062592	1.849377	1.777274	H	-0.688589	0.131372	2.503865
H	2.573089	0.198157	2.234838	C	-3.353042	-0.026185	3.239471
C	0.854556	-2.891206	0.381346	H	-2.785913	-0.936111	3.477596
C	2.384188	-3.099601	0.284486	H	-3.347276	0.627193	4.124201
H	2.911010	-2.204067	0.638779	H	-4.391768	-0.321954	3.056753
H	2.715702	-3.951798	0.893337	H	-3.279033	1.638548	1.897268

Table 2 (continued).



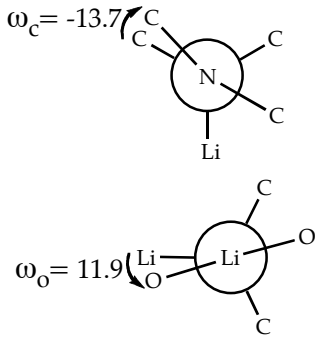


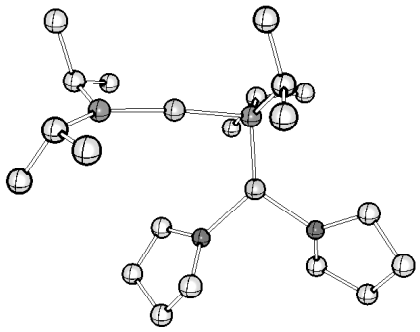
4f
G = -1063.120314
G_{MP2} = -1059.325333
ΔG = 9.5 kcal/mol
ΔG_{MP2} = 11.6 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	-2.573179	0.747003	2.056481	H	2.667385	-3.326237	-0.814948
N	-2.720673	-0.065884	0.860757	C	0.519841	-2.584895	1.817128
Li	-1.451567	-1.247665	0.169199	H	-0.562935	-2.545081	1.995585
N	0.304397	-1.903488	-0.558130	H	0.938342	-3.330948	2.503943
Li	1.072551	-0.074862	-0.492683	H	0.937020	-1.607698	2.098031
O	0.411867	1.676606	-1.107095	H	0.390488	-3.908274	0.157752
C	1.201913	2.888719	-1.105183	C	0.202052	-2.437410	-1.928926
C	0.290083	3.991327	-1.652616	C	-1.002453	-3.382995	-2.142581
C	-1.106175	3.486090	-1.258521	H	-1.949165	-2.832264	-2.060123
C	-0.971690	1.981050	-1.465294	H	-0.977180	-3.852972	-3.135231
H	-1.120727	1.707222	-2.517765	H	-1.016953	-4.187431	-1.398761
H	-1.621880	1.373664	-0.822231	C	0.130001	-1.299098	-2.956539
H	-1.908256	3.917424	-1.864227	H	1.034609	-0.674599	-2.934624
H	-1.316961	3.708033	-0.206058	H	0.024445	-1.686239	-3.977311
H	0.378214	4.054557	-2.743571	H	-0.732964	-0.650175	-2.758752
H	0.534707	4.973183	-1.235939	H	1.103578	-3.026329	-2.184527
H	1.512793	3.096750	-0.074116	C	-4.101236	-0.154088	0.406006
H	2.097681	2.727079	-1.713662	C	-4.268368	-1.343808	-0.550427
O	2.847890	0.477261	0.225551	H	-4.005656	-2.286144	-0.051517
C	4.101837	0.257038	-0.466713	H	-5.296941	-1.432350	-0.922512
C	5.175012	0.222065	0.622949	H	-3.616117	-1.224153	-1.429307
C	4.582949	1.154222	1.691911	C	-4.620197	1.126936	-0.294715
C	3.093191	0.820894	1.612714	H	-4.085780	1.289943	-1.240851
H	2.435325	1.653585	1.876933	H	-5.694089	1.062231	-0.520776
H	2.836464	-0.043225	2.237209	H	-4.469614	2.012867	0.332899
H	4.756870	2.203604	1.426551	H	-4.798910	-0.342084	1.247970
H	4.993787	0.982585	2.690827	C	-1.099312	1.129947	2.270119
H	6.151634	0.548875	0.254599	H	-0.702980	1.674067	1.404431
H	5.281431	-0.793985	1.019347	H	-0.968714	1.757019	3.161937
H	4.020374	-0.676308	-1.030703	H	-0.489682	0.226429	2.413003
H	4.261065	1.086552	-1.167860	C	-3.095299	0.069288	3.348057

Table 2 (continued).

C	0.850722	-2.921766	0.356325	H	-2.507843	-0.833716	3.561948
C	2.377689	-3.129758	0.223626	H	-3.030633	0.739120	4.218076
H	2.911588	-2.231780	0.560734	H	-4.142731	-0.233932	3.244544
H	2.725458	-3.978213	0.828735	H	-3.127919	1.707048	1.971934



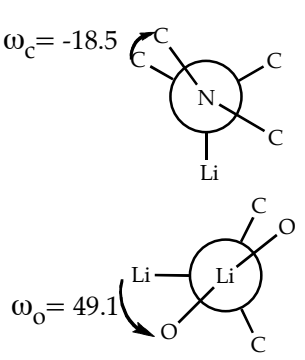


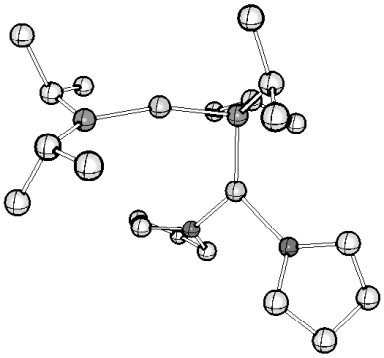
4g
G = -1063.121261
G_{MP2} = -1059.324248
ΔG = 8.9 kcal/mol
ΔG_{MP2} = 12.3 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	4.239235	-0.301231	-0.707950	H	-1.651012	-4.123563	-0.809332
N	3.152230	0.059435	0.190363	C	-0.206983	-1.437550	-2.479179
Li	1.535220	-0.859754	0.128198	H	0.675276	-0.795547	-2.377779
N	-0.288367	-1.704288	-0.043741	H	-0.134737	-1.950044	-3.445801
Li	-1.327303	-0.063266	-0.093525	H	-1.097487	-0.789644	-2.522360
O	-3.277589	0.114987	0.052386	H	0.553352	-3.121993	-1.418478
C	-4.106565	1.029949	-0.692724	C	-0.479893	-2.556700	1.138443
C	-5.492619	1.010064	-0.004726	C	0.638560	-3.599124	1.362795
C	-5.395597	-0.162767	1.005802	H	1.609192	-3.106245	1.517270
C	-4.151450	-0.921015	0.541589	H	0.434511	-4.221364	2.244116
H	-4.379870	-1.620367	-0.274909	H	0.741346	-4.270123	0.502875
H	-3.618164	-1.456963	1.328106	C	-0.608789	-1.675380	2.390945
H	-6.288504	-0.794220	1.010083	H	-1.447484	-0.968566	2.302894
H	-5.244240	0.215034	2.021871	H	-0.784414	-2.279624	3.289205
H	-6.284527	0.844634	-0.740999	H	0.302105	-1.087549	2.560695
H	-5.707074	1.955416	0.501038	H	-1.424592	-3.131954	1.071108
H	-3.610703	2.002076	-0.675963	C	3.595759	0.905832	1.283971
H	-4.171032	0.685641	-1.733758	C	2.583067	0.868134	2.436938
O	-0.701246	1.771197	-0.315600	H	2.499876	-0.145390	2.848067
C	-0.909435	2.840205	0.626381	H	2.859726	1.546795	3.254380
C	-0.747835	4.107892	-0.206616	H	1.587482	1.172576	2.077326
C	0.419885	3.730202	-1.139807	C	3.842938	2.381916	0.879667
C	0.311137	2.197639	-1.282267	H	2.895203	2.862741	0.600683
H	1.253600	1.685779	-1.050902	H	4.291045	2.963412	1.698610
H	-0.048615	1.883190	-2.265787	H	4.516160	2.449899	0.017973
H	1.376950	3.997922	-0.681612	H	4.556476	0.549971	1.711910

Table 2 (continued).

H	0.361195	4.238105	-2.106587	C	3.684339	-0.779817	-2.057327
H	-0.537725	4.990021	0.405443	H	3.088601	0.007048	-2.535570
H	-1.662544	4.298846	-0.780285	H	4.485152	-1.073648	-2.748060
H	-1.902831	2.705086	1.063882	H	3.038494	-1.661109	-1.920469
H	-0.156141	2.783999	1.423735	C	5.178140	-1.393343	-0.137939
C	-0.316613	-2.439636	-1.318945	H	4.622792	-2.332041	-0.005501
C	-1.564804	-3.320160	-1.548106	H	6.034297	-1.588274	-0.800263
H	-2.480137	-2.713394	-1.492195	H	5.577682	-1.104077	0.840559
H	-1.530695	-3.791042	-2.538773	H	4.887043	0.571453	-0.936778



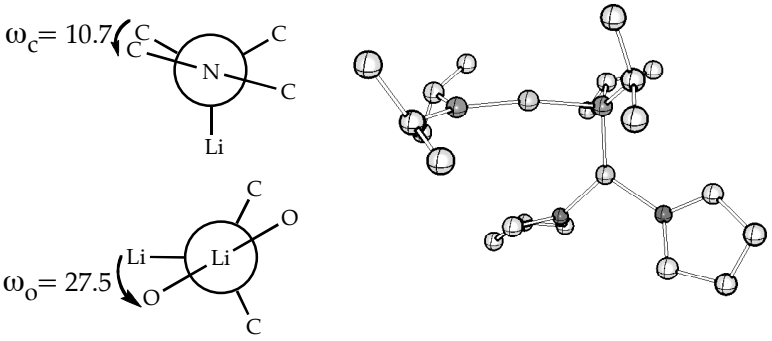


4h
G = -1063.119726
G_{MP2} = -1059.322855
ΔG = 9.9 kcal/mol
ΔG_{MP2} = 13.2 kcal/mol

Atom	X	Y	Z	Atom	X	Y	Z
C	3.068149	-0.324413	-2.138269	H	-2.357427	2.554031	2.174782
N	2.962459	-0.054140	-0.711733	C	0.406735	0.583922	2.932637
Li	1.617746	0.962670	0.107801	H	1.487757	0.621136	2.761031
N	-0.151934	1.665676	0.770461	H	0.239906	0.603136	4.016936
Li	-1.201055	0.142133	0.105035	H	0.044641	-0.382140	2.555674
O	-0.853890	-1.780161	0.340838	H	0.137695	2.674133	2.627359
C	-1.730396	-2.660724	1.065267	C	-0.372442	2.984898	0.148964
C	-0.828077	-3.422781	2.052990	C	0.842126	3.933352	0.282297
C	0.593589	-3.297266	1.437018	H	1.699861	3.548776	-0.288632
C	0.375579	-2.521850	0.130257	H	0.616532	4.939521	-0.096834
H	0.222902	-3.202345	-0.719576	H	1.156053	4.036882	1.327130
H	1.169284	-1.805393	-0.114320	C	-0.734198	2.839854	-1.336265
H	1.057482	-4.269675	1.249408	H	-1.651003	2.251815	-1.467757
H	1.254595	-2.737367	2.104437	H	-0.891850	3.818321	-1.806542
H	-1.150903	-4.462673	2.159230	H	0.067987	2.335703	-1.888805
H	-0.863496	-2.962487	3.044469	H	-1.224836	3.504246	0.628666
H	-2.499406	-2.046722	1.540544	C	4.209105	-0.325851	-0.008766
H	-2.215027	-3.347815	0.355871	C	3.967090	-0.419153	1.503922
O	-3.004993	0.036645	-0.692646	H	3.231203	-1.197983	1.738021
C	-4.099119	0.964568	-0.569730	H	4.891502	-0.642030	2.051724

Table 2 (continued).

C	-5.345452	0.115094	-0.837062	H	3.586651	0.537865	1.893051
C	-4.842134	-0.964966	-1.833628	C	5.317277	0.726419	-0.263604
C	-3.306710	-0.792683	-1.833751	H	5.009531	1.700752	0.140449
H	-2.959386	-0.284629	-2.743462	H	6.268256	0.441994	0.209721
H	-2.746567	-1.720937	-1.711380	H	5.509452	0.857494	-1.334063
H	-5.248441	-0.816497	-2.838120	H	4.640926	-1.304185	-0.308531
H	-5.131841	-1.967352	-1.506765	C	1.929942	0.364191	-2.901798
H	-6.168813	0.711741	-1.239607	H	1.983256	1.452518	-2.777549
H	-5.691169	-0.348890	0.091868	H	1.960425	0.141335	-3.976146
H	-4.047444	1.401482	0.428702	H	0.953436	0.023242	-2.522734
H	-3.983708	1.762695	-1.316569	C	3.077529	-1.830993	-2.506124
C	-0.313373	1.744431	2.233533	H	2.103231	-2.288546	-2.289488
C	-1.794629	1.763888	2.685222	H	3.292295	-1.985346	-3.573273
H	-2.280349	0.801235	2.458542	H	3.837331	-2.376753	-1.935610
H	-1.893169	1.933155	3.766170	H	4.006422	0.089897	-2.561827

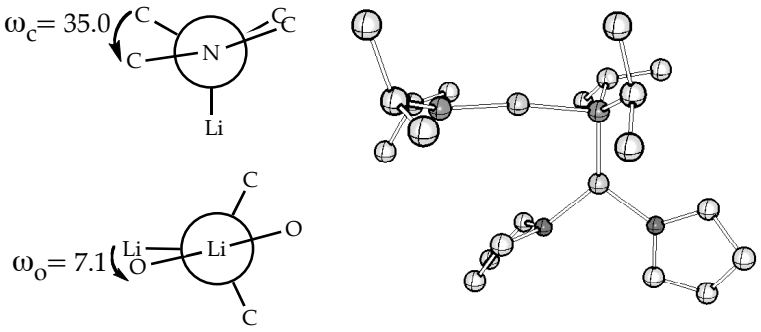


4i
G = -1063.120663
G_{MP2} = -1059.324724
ΔG = 9.3 kcal/mol
ΔG_{MP2} = 12.0 kcal/mol
(example of heterochiral form)

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.529909	-0.237119	-1.835938	H	1.881984	-1.523996	-1.686577
N	-3.028684	-0.331829	-0.474045	C	-0.167800	-3.834433	-0.074133
Li	-1.403610	-1.045648	0.077089	H	-0.347463	-4.159861	0.956593
N	0.488343	-1.491439	0.641564	H	0.176936	-4.708934	-0.641587
Li	1.323260	0.202957	0.166197	H	-1.135112	-3.525424	-0.496962
O	3.227788	0.455816	-0.240753	H	1.818488	-3.110452	0.221333
C	4.213830	-0.569054	0.046023	C	0.401374	-1.729990	2.093750
C	5.205626	-0.505431	-1.113321	C	0.238115	-0.382069	2.814858
C	5.210112	0.995806	-1.441874	H	1.169775	0.202326	2.755687
C	3.742463	1.381364	-1.232192	H	0.008035	-0.519069	3.878077
H	3.154648	1.261791	-2.150428	H	-0.566069	0.217538	2.371812
H	3.606282	2.400223	-0.859520	C	1.603167	-2.470365	2.719178
H	5.555140	1.217220	-2.455893	H	1.706232	-3.493386	2.343820

Table 2 (continued).

H	5.853324	1.537625	-0.738763	H	1.492032	-2.532508	3.808994
H	4.833816	-1.085171	-1.966050	H	2.539528	-1.936555	2.503476
H	6.191948	-0.891783	-0.840879	H	-0.492425	-2.334502	2.359092
H	4.696530	-0.333872	1.003431	C	-4.044664	0.012198	0.510276
H	3.684813	-1.519635	0.138555	C	-3.748983	-0.660416	1.859545
O	0.638650	2.034834	0.046550	H	-3.739250	-1.752013	1.752736
C	0.998813	3.031507	1.025187	H	-4.491179	-0.395034	2.623812
C	-0.299600	3.773888	1.324983	H	-2.767338	-0.345846	2.244720
C	-0.963950	3.814801	-0.061137	C	-4.204796	1.538639	0.724306
C	-0.552811	2.474284	-0.685151	H	-3.296554	1.952289	1.185319
H	-0.285733	2.564526	-1.743386	H	-5.056474	1.781147	1.376650
H	-1.320818	1.699500	-0.568290	H	-4.361808	2.051218	-0.232301
H	-0.573492	4.656699	-0.644483	H	-5.044295	-0.354552	0.204014
H	-2.051298	3.913680	-0.006354	C	-2.372432	-0.236263	-2.844617
H	-0.127594	4.766364	1.752359	H	-1.682759	0.596117	-2.662608
H	-0.909484	3.195300	2.027662	H	-2.734560	-0.159761	-3.877746
H	1.429467	2.515135	1.887753	H	-1.802991	-1.173687	-2.768380
H	1.757407	3.705889	0.600995	C	-4.505718	-1.376945	-2.223582
C	0.860890	-2.681785	-0.135765	H	-3.979604	-2.340669	-2.199684
C	1.095167	-2.286039	-1.601749	H	-4.922362	-1.233827	-3.231344
H	0.183124	-1.874889	-2.053513	H	-5.348161	-1.442398	-1.526415
H	1.401563	-3.149138	-2.205161	H	-4.085688	0.712663	-2.001332



4j
G = -1063.12036
G_{MP2} = -1059.324244
ΔG = 9.5 kcal/mol
ΔG_{MP2} = 12.3 kcal/mol
(example of heterochiral form)

Atom	X	Y	Z	Atom	X	Y	Z
C	-3.822883	-0.419648	-1.400362	H	1.768704	-1.078627	-1.925176
N	-3.079414	-0.194724	-0.167119	C	-0.230629	-3.715896	-0.822635
Li	-1.423501	-0.997980	0.185830	H	-0.333991	-4.299482	0.098911
N	0.494753	-1.636388	0.432405	H	0.061938	-4.408902	-1.622504
Li	1.378233	0.086923	0.223731	H	-1.223220	-3.316078	-1.073411
O	3.284970	0.433162	-0.021492	H	1.776748	-3.076749	-0.488672

Table 2 (continued).

C	4.280447	-0.622899	-0.045559	C	0.545412	-2.242670	1.774726
C	5.385514	-0.113282	-0.968939	C	0.394887	-1.136430	2.829624
C	5.345386	1.399993	-0.705116	H	1.263171	-0.458931	2.808914
C	3.845295	1.661546	-0.551559	H	0.329424	-1.552043	3.842238
H	3.368124	1.870826	-1.516521	H	-0.506374	-0.537219	2.659974
H	3.607677	2.474751	0.138957	C	1.821653	-3.051316	2.094275
H	5.789128	1.993207	-1.509838	H	1.933718	-3.928284	1.448707
H	5.874098	1.639167	0.224921	H	1.798980	-3.411290	3.130518
H	5.140019	-0.327452	-2.015675	H	2.717468	-2.426309	1.972529
H	6.355745	-0.566482	-0.746499	H	-0.299735	-2.945156	1.938907
H	4.647012	-0.780803	0.976266	C	-3.918676	0.412652	0.855019
H	3.790783	-1.536379	-0.389881	C	-3.341363	0.176009	2.256617
O	0.582813	1.876776	0.069088	H	-3.248088	-0.897348	2.464333
C	0.206246	2.654966	1.224164	H	-3.965738	0.624623	3.040061
C	-0.282713	4.010505	0.675985	H	-2.341835	0.628564	2.341997
C	-0.561939	3.737657	-0.827436	C	-4.144609	1.933988	0.656459
C	-0.370561	2.223272	-0.972830	H	-3.199581	2.479746	0.787256
H	0.073891	1.919676	-1.924373	H	-4.872997	2.340130	1.373318
H	-1.301901	1.663369	-0.804563	H	-4.516753	2.150089	-0.351344
H	0.150274	4.282481	-1.455150	H	-4.931425	-0.040223	0.867120
H	-1.570461	4.037574	-1.124993	C	-2.873787	-0.596200	-2.593633
H	0.478721	4.786282	0.798850	H	-2.231173	0.283282	-2.721465
H	-1.179946	4.339822	1.207192	H	-3.423842	-0.757863	-3.529587
H	-0.593258	2.132962	1.763567	H	-2.227006	-1.472407	-2.445222
H	1.085656	2.726644	1.870035	C	-4.770280	-1.643844	-1.337054
C	0.801132	-2.578349	-0.654485	H	-4.183805	-2.564907	-1.216386
C	0.947097	-1.808172	-1.977300	H	-5.381338	-1.740044	-2.246627
H	0.028261	-1.262998	-2.226582	H	-5.455850	-1.574388	-0.485089
H	1.166359	-2.484405	-2.812448	H	-4.465192	0.451733	-1.648788

Table 3. Optimized geometries of THF trisolvated LDA open dimers at the B3LYP level of theory with 6-31G(d) basis set at -78 °C with free energies (Hartrees) and cartesian coordinates (X, Y, Z). Single point MP2 energies are included. A representative image is shown below. Dihedral angles ω_C and ω_O are included as described in Table 2. The connectivity of transition states and ground states is indicated beneath the energy values. Comments on geometry are included where deemed appropriate.

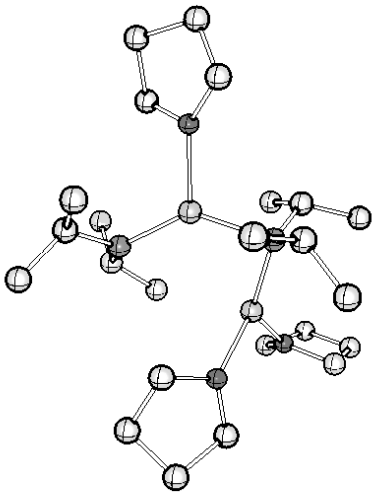
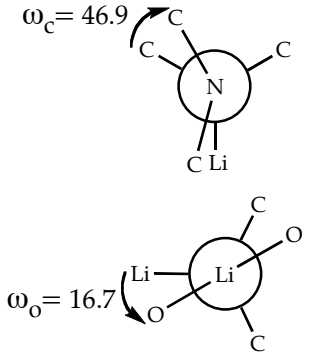
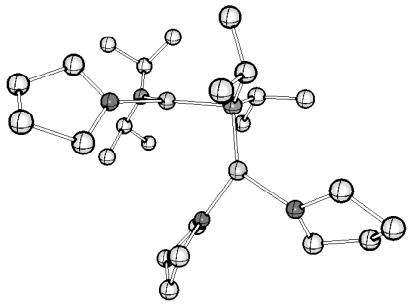


Table 3 (continued).



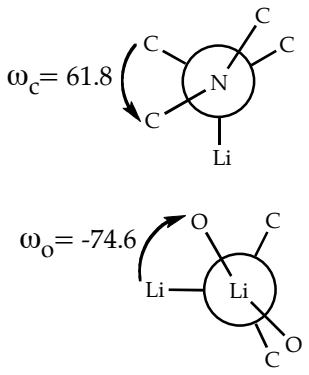


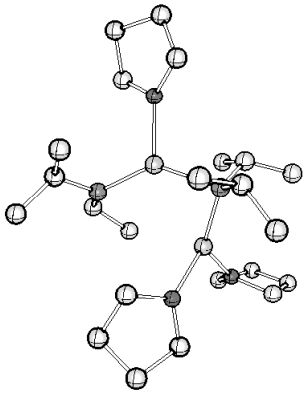
5a
G = -1295.455989
G_{MP2} = -1290.892445
ΔG = 18.1 kcal/mol
ΔG_{MP2} = 13.3 kcal/mol
11 → 5a → 13

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.681747	-2.299236	-1.269863	C	3.836154	0.987902	3.081800
N	-0.542337	-1.581315	0.010766	C	3.296494	-0.181790	2.254925
Li	-1.737316	-0.049876	0.023742	H	3.301533	-1.118334	2.828357
O	-3.700877	-0.067842	0.401335	H	3.801023	-0.327885	1.296348
C	-4.630134	0.562804	-0.510872	H	4.610742	0.675618	3.788869
C	-5.801092	-0.410199	-0.639506	H	4.265467	1.754330	2.426057
C	-5.847995	-1.034253	0.763636	H	2.321276	0.912078	4.646042
C	-4.363737	-1.144192	1.122223	H	2.650657	2.564261	4.088833
H	-3.926028	-2.090800	0.791229	H	1.500577	2.182873	1.983897
H	-4.161739	-1.014588	2.188740	H	0.506336	1.164840	3.061471
H	-6.350752	-2.005217	0.787057	C	-1.780247	2.881565	0.633442
H	-6.366823	-0.366796	1.461683	C	-1.929160	4.203730	-0.121517
H	-5.578694	-1.175246	-1.391967	C	-1.033205	3.974970	-1.348855
H	-6.730932	0.090892	-0.924097	C	-1.286723	2.501703	-1.663930
H	-4.949334	1.524497	-0.086969	H	-0.435103	1.993970	-2.119809
H	-4.107317	0.751217	-1.452586	H	-2.169258	2.370246	-2.304329
O	-1.553972	1.873037	-0.381742	H	0.020397	4.128942	-1.092360
Li	1.389419	-0.645826	-0.016374	H	-1.279396	4.627209	-2.191647
N	2.878329	-0.228701	-1.194989	H	-1.624725	5.062330	0.484027
C	3.754425	-1.232399	-1.779363	H	-2.970804	4.356688	-0.428215
H	3.830934	-1.124280	-2.884370	H	-2.668595	2.595396	1.204922
C	5.214729	-1.179277	-1.257084	H	-0.914244	2.896029	1.306030
H	5.637419	-0.172016	-1.347399	C	-0.698948	-2.464036	1.175645
H	5.249756	-1.462817	-0.196012	H	-1.628574	-3.064373	1.103570
H	5.873193	-1.864488	-1.811322	C	0.443067	-3.488612	1.362634
C	3.202071	-2.643177	-1.535136	H	0.572467	-4.114201	0.473360
H	2.221707	-2.769192	-2.006842	H	1.396034	-2.975573	1.549363
H	3.873678	-3.417386	-1.929038	H	0.247141	-4.156655	2.212671
H	3.084582	-2.827401	-0.457077	C	-0.835940	-1.635307	2.462681
C	3.140482	1.091305	-1.736714	H	-1.676164	-0.927204	2.399977
H	4.229507	1.298677	-1.822793	H	-1.019477	-2.279586	3.332203

Table 3 (continued).

C	2.591261	2.181375	-0.802495	H	0.078553	-1.063778	2.645328
H	1.521087	2.011752	-0.607475	H	0.099350	-3.075213	-1.385813
H	3.109168	2.163116	0.162372	C	-0.478166	-1.316406	-2.431250
H	2.700690	3.186374	-1.234095	H	-0.535849	-1.826977	-3.400734
C	2.571159	1.319659	-3.163088	H	-1.264317	-0.541632	-2.431145
H	2.880056	2.288704	-3.583920	H	0.497568	-0.822214	-2.358892
H	2.910351	0.537308	-3.850796	C	-2.028954	-3.033812	-1.477931
H	1.472789	1.285353	-3.149446	H	-2.056334	-3.523880	-2.459793
O	1.914860	0.149780	1.950430	H	-2.208554	-3.809120	-0.725350
C	1.517619	1.325880	2.671704	H	-2.868064	-2.322411	-1.435257
C	2.568371	1.520798	3.767981				



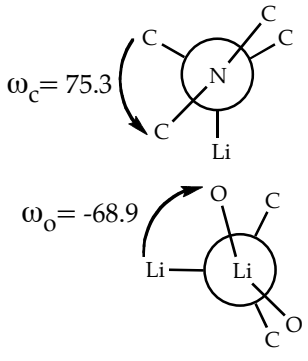


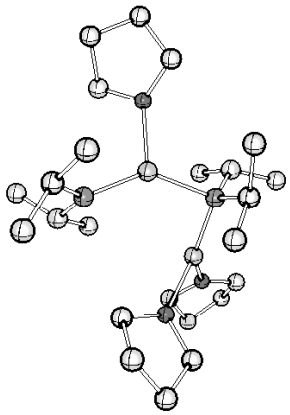
5b
G = -1295.464704
G_{MP2} = -1290.904916
$\Delta G^{\ddagger}$ = 12.2 kcal/mol
$\Delta G_{MP2}^{\ddagger}$ = 5.5 kcal/mol
5b → 14
(geometry akin to **4**)

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.915659	1.893773	2.086103	H	0.297605	2.434192	-0.678429
N	-1.442740	1.663085	0.750524	H	0.984858	2.653581	-2.330595
Li	-1.409317	-0.106153	-0.103283	H	1.909821	4.030927	0.248068
O	-3.200214	-1.152075	0.009106	H	1.581972	4.799225	-1.316040
C	-4.120889	-0.827099	1.079410	H	4.171297	4.123534	-0.731034
C	-5.507468	-1.203883	0.556493	H	3.535807	3.747169	-2.340189
C	-5.188165	-2.397050	-0.357487	H	4.079941	1.504216	-1.731045
C	-3.859653	-1.966750	-0.983939	H	3.925082	1.844944	0.008376
H	-3.200390	-2.800969	-1.238567	O	3.234056	-0.790045	0.647088
H	-4.022254	-1.360298	-1.885307	C	4.258464	-1.558999	-0.009762
H	-5.054318	-3.308609	0.237246	C	4.750051	-2.589672	1.030853
H	-5.960058	-2.591526	-1.108424	C	4.170070	-2.075305	2.375830
H	-6.205958	-1.447859	1.362658	C	3.629927	-0.684636	2.024831
H	-5.933889	-0.379285	-0.026978	H	2.753888	-0.377977	2.597835
H	-3.994318	0.230577	1.315366	H	4.409299	0.086620	2.121394
H	-3.851607	-1.420450	1.963457	H	3.352513	-2.719686	2.712091
C	-2.512963	2.591249	0.408105	H	4.917451	-2.035459	3.173589

Table 3 (continued).

C	-3.140284	2.206898	-0.941800	H	4.379160	-3.592255	0.802051
H	-3.526504	1.181373	-0.924945	H	5.843030	-2.636312	1.045116
H	-3.969127	2.876766	-1.204960	H	5.069539	-0.883759	-0.317124
H	-2.391700	2.270047	-1.742532	H	3.809252	-2.002013	-0.900406
C	-2.098184	4.084604	0.324714	C	-0.106312	-2.678801	-0.293255
H	-1.371258	4.237198	-0.484348	C	0.940462	-3.753429	-0.674938
H	-2.967684	4.725472	0.122336	H	1.944728	-3.447964	-0.351333
H	-1.642804	4.441830	1.254549	H	0.708823	-4.716300	-0.198047
H	-3.348497	2.565541	1.149093	H	0.971246	-3.924793	-1.755613
C	0.451191	1.209587	2.247713	C	-0.156833	-2.573927	1.237448
H	1.172034	1.611750	1.525172	H	-0.944917	-1.889518	1.570900
H	0.862258	1.353157	3.256605	H	-0.352229	-3.552387	1.694210
H	0.354849	0.127508	2.082273	H	0.800028	-2.208667	1.634791
C	-1.843117	1.423185	3.236877	H	-1.083775	-3.108808	-0.606421
H	-1.960210	0.330893	3.211776	C	-0.026881	-1.416343	-2.367599
H	-1.447844	1.700544	4.225231	C	-0.885853	-0.265141	-2.922368
H	-2.840497	1.869092	3.147325	H	-0.477021	0.705250	-2.615358
H	-0.728425	2.970124	2.280740	H	-0.927525	-0.275954	-4.019833
N	0.075805	-1.355492	-0.898410	H	-1.916822	-0.323532	-2.553953
Li	1.534677	-0.188477	-0.278696	C	1.337903	-1.399430	-3.101379
O	2.139438	1.551517	-0.988125	H	1.989448	-2.206173	-2.750011
C	3.496739	2.048597	-0.979506	H	1.221235	-1.510545	-4.189119
C	3.406642	3.554539	-1.268881	H	1.852941	-0.444754	-2.922522
C	1.970687	3.895183	-0.838133	H	-0.532797	-2.354141	-2.668222
C	1.210217	2.641853	-1.255048				





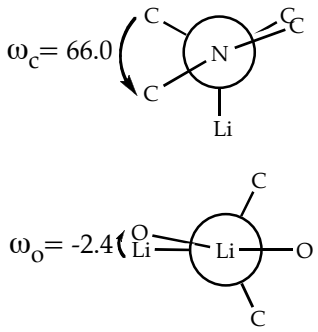
5c
G = -1295.463115
G_{MP2} = -1290.902852
$\Delta G^{\ddagger}$ = 13.7 kcal/mol
$\Delta G_{MP2}^{\ddagger}$ = 6.8 kcal/mol
12 → 5c
(geometry akin to **4**)

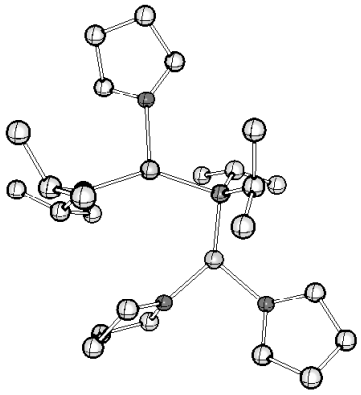
Atom	X	Y	Z	Atom	X	Y	Z
C	0.898529	2.043246	-1.964721	C	1.540648	-1.407695	3.108066
N	1.477419	1.642439	-0.695006	H	2.229730	-0.654568	2.702943
Li	1.394719	-0.134025	0.109705	H	1.572665	-1.335040	4.203618
N	-0.040172	-1.336370	1.117720	H	1.923739	-2.396780	2.834891

Table 3 (continued).

Li	-1.608175	-0.447628	0.337012	C	-0.373866	0.205858	3.017908
O	-2.454766	1.353267	0.504322	H	-1.441755	0.341601	2.807519
C	-1.717823	2.597663	0.344702	H	-0.228477	0.349584	4.095831
C	-2.108973	3.422782	1.563883	H	0.173904	0.997222	2.491322
C	-3.597267	3.064613	1.725907	H	-0.530787	-1.906875	3.118180
C	-3.653825	1.593286	1.274636	O	3.161618	-1.216474	-0.341585
H	-3.651262	0.899755	2.123831	C	3.897380	-0.693132	-1.471511
H	-4.531217	1.375650	0.653998	C	5.365715	-0.799730	-1.070386
H	-3.965072	3.195232	2.747970	C	5.373829	-2.118149	-0.280218
H	-4.211356	3.689661	1.067594	C	4.015235	-2.085626	0.436738
H	-1.532877	3.102110	2.438779	H	3.546458	-3.072253	0.510954
H	-1.941842	4.493608	1.415953	H	4.096275	-1.665754	1.445335
H	-2.046919	3.083437	-0.584493	H	5.426077	-2.970500	-0.967937
H	-0.655916	2.336648	0.259858	H	6.209736	-2.201496	0.421223
O	-3.178342	-1.209090	-0.705634	H	6.039756	-0.808101	-1.932567
C	-3.962795	-2.408741	-0.487846	H	5.644565	0.040749	-0.424073
C	-4.933546	-2.503768	-1.671459	H	3.523801	0.318545	-1.636781
C	-5.068109	-1.037898	-2.112357	H	3.684419	-1.310443	-2.357245
C	-3.651846	-0.516081	-1.885004	C	2.405523	2.617628	-0.139960
H	-2.993504	-0.756859	-2.729864	C	3.032477	2.066678	1.150389
H	-3.588530	0.554360	-1.681206	H	3.523168	1.102834	0.966725
H	-5.393877	-0.926492	-3.150740	H	3.782606	2.754301	1.561909
H	-5.780491	-0.505121	-1.470951	H	2.263229	1.914676	1.919880
H	-4.496175	-3.102868	-2.478306	C	1.805055	4.012444	0.167403
H	-5.885745	-2.962404	-1.389494	H	1.032357	3.936332	0.944625
H	-4.490490	-2.299341	0.467257	H	2.576455	4.707672	0.526621
H	-3.283853	-3.262004	-0.416939	H	1.345966	4.464191	-0.719377
C	0.198782	-2.718093	0.674371	H	3.262761	2.815185	-0.823277
C	-0.694873	-3.789855	1.342783	C	-0.030683	0.934247	-2.479426
H	-1.757555	-3.536542	1.227767	H	-0.813720	0.711401	-1.743422
H	-0.526334	-4.777919	0.894361	H	-0.524847	1.217678	-3.418139
H	-0.496989	-3.884080	2.415653	H	0.534699	0.009990	-2.659470
C	0.041211	-2.809834	-0.851369	C	1.904592	2.389832	-3.093279
H	0.724441	-2.122125	-1.362011	H	2.524393	1.518957	-3.345959
H	0.260492	-3.822769	-1.212267	H	1.379549	2.706589	-4.005033
H	-0.982359	-2.558281	-1.159874	H	2.577115	3.204770	-2.805202
H	1.239829	-3.036863	0.885463	H	0.255109	2.951408	-1.873819
C	0.106329	-1.182645	2.574487				

Table 3 (continued).



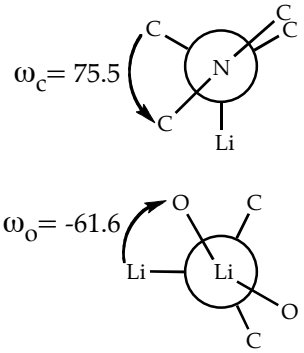


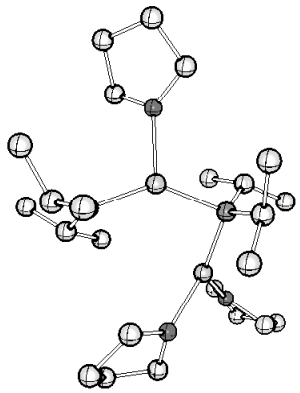
5d
G = -1295.458203
G_{MP2} = -1290.897229
ΔG = 16.7 kcal/mol
ΔG_{MP2} = 10.3 kcal/mol
(distorted diisopropyl-amido geometry)

Atom	X	Y	Z	Atom	X	Y	Z
C	1.965915	2.558584	-0.629722	C	0.419086	-3.005458	1.767022
N	1.946855	1.526908	0.388941	H	1.249523	-2.328689	2.009196
Li	1.315998	-0.306774	0.066784	H	0.120529	-3.518731	2.691123
N	-0.462082	-1.517097	-0.101833	H	0.794215	-3.770130	1.078514
Li	-1.914866	-0.209557	-0.355474	C	-1.306298	-1.236472	2.196275
O	-3.894148	-0.624685	-0.297971	H	-2.254568	-0.781294	1.874403
C	-4.890382	0.365885	0.042944	H	-1.502574	-1.733809	3.154243
C	-5.826328	-0.334604	1.022902	H	-0.587536	-0.430223	2.377332
C	-5.867953	-1.757170	0.443501	H	-1.564992	-2.983571	1.006196
C	-4.435414	-1.956154	-0.071657	O	3.048988	-1.477754	-0.419943
H	-3.793418	-2.451713	0.662602	C	4.192904	-0.727564	-0.865849
H	-4.389394	-2.515965	-1.009034	C	5.395889	-1.412829	-0.201561
H	-6.149190	-2.515628	1.179623	C	4.915173	-2.875198	0.010947
H	-6.586098	-1.808399	-0.382981	C	3.450440	-2.851878	-0.473545
H	-5.389336	-0.338215	2.028266	H	3.371335	-3.214574	-1.509794
H	-6.810574	0.139985	1.077616	H	2.765949	-3.423624	0.152645
H	-5.423802	0.671209	-0.868414	H	5.508741	-3.599976	-0.555183
H	-4.363492	1.229637	0.450941	H	4.973011	-3.155579	1.067059
O	-2.046593	1.742062	-0.413040	H	6.294080	-1.349273	-0.823649
C	-2.420150	2.598901	-1.515577	H	5.619944	-0.935889	0.757294
C	-1.765952	3.953746	-1.235165	H	4.014666	0.304053	-0.563115
C	-1.711212	3.984545	0.300301	H	4.257108	-0.790792	-1.964169
C	-1.414071	2.526626	0.649565	C	2.403399	2.004139	1.687756
H	-0.344612	2.280668	0.652403	C	3.908042	1.761486	1.989001
H	-1.862048	2.210639	1.597524	H	4.553501	2.180983	1.212585
H	-0.939908	4.658145	0.683010	H	4.209261	2.200867	2.951923
H	-2.677955	4.298516	0.713979	H	4.105630	0.681710	2.039221
H	-0.752589	3.978627	-1.646705	C	1.601477	1.353304	2.831220
H	-2.335603	4.783347	-1.664996	H	1.701802	0.258987	2.788775
H	-3.515884	2.674404	-1.544384	H	1.957614	1.673705	3.819803
H	-2.075856	2.135426	-2.445449	H	0.535457	1.594596	2.759021
C	-0.221610	-2.429224	-1.230844	H	2.238168	3.100445	1.779147

Table 3 (continued).

C	-1.433667	-3.292579	-1.656487	C	1.406818	1.999395	-1.947266
H	-2.244048	-2.655687	-2.039336	H	0.420601	1.546183	-1.791771
H	-1.155869	-3.992811	-2.455542	H	1.312363	2.779249	-2.714816
H	-1.833187	-3.887960	-0.828482	H	2.071194	1.222980	-2.349344
C	0.245659	-1.629014	-2.454992	C	3.325628	3.241439	-0.937316
H	1.189444	-1.109572	-2.262975	H	4.068491	2.509942	-1.282617
H	0.396209	-2.282521	-3.323572	H	3.210530	4.002993	-1.722546
H	-0.504134	-0.874394	-2.735368	H	3.733150	3.745308	-0.055398
H	0.589773	-3.148509	-1.003318	H	1.300839	3.418065	-0.345512
C	-0.765600	-2.226543	1.149878				





5e
G = -1295.461125
G_{MP2} = -1290.900545
ΔG = 14.9 kcal/mol
ΔG_{MP2} = 8.3 kcal/mol
(distorted diisopropyl-amido geometry)

Atom	X	Y	Z	Atom	X	Y	Z
C	1.063602	2.382851	-1.371190	C	1.230290	-2.201977	2.806660
N	1.651651	1.659754	-0.263044	H	1.984574	-1.418184	2.651615
Li	1.373630	-0.219289	0.182878	H	1.200541	-2.431178	3.880548
N	-0.211854	-1.473457	0.844015	H	1.568444	-3.106754	2.290319
Li	-1.660635	-0.227094	0.356211	C	-0.585209	-0.502201	3.090433
O	-3.412935	-0.789480	-0.518473	H	-1.616133	-0.206361	2.852917
C	-4.478871	-1.269065	0.338866	H	-0.540106	-0.692682	4.169995
C	-5.436816	-2.038532	-0.575195	H	0.068955	0.350291	2.874048
C	-5.233070	-1.337222	-1.927686	H	-0.858801	-2.543734	2.577758
C	-3.732809	-1.047009	-1.906111	O	3.093866	-1.308096	-0.376745
H	-3.149479	-1.909484	-2.250432	C	3.779387	-0.862617	-1.559840
H	-3.439399	-0.168451	-2.487891	C	5.261954	-1.182828	-1.306837
H	-5.526039	-1.952970	-2.782945	C	5.218970	-2.339459	-0.269247
H	-5.805157	-0.402713	-1.967217	C	3.713288	-2.549023	-0.017011
H	-5.137528	-3.090475	-0.643201	H	3.311950	-3.354311	-0.651051
H	-6.470098	-2.001240	-0.218317	H	3.457874	-2.758680	1.021919
H	-4.963883	-0.400101	0.800832	H	5.693806	-3.254552	-0.636670
H	-4.035371	-1.887320	1.124735	H	5.729041	-2.050433	0.654566

Table 3 (continued).

O	-2.250754	1.611036	0.849502	H	5.775953	-1.465418	-2.230767
C	-3.400880	2.312855	0.347949	H	5.775406	-0.310013	-0.893344
C	-2.860215	3.663694	-0.110487	H	3.543015	0.195107	-1.673955
C	-1.827806	3.974689	0.986901	H	3.396330	-1.423287	-2.427572
C	-1.301801	2.585023	1.393344	C	2.542353	2.483620	0.545919
H	-0.324377	2.336838	0.963791	C	4.047212	2.413015	0.165214
H	-1.268079	2.457877	2.480087	H	4.214098	2.634249	-0.892200
H	-1.021782	4.622867	0.633839	H	4.650969	3.117480	0.756828
H	-2.313940	4.471013	1.834931	H	4.428481	1.401886	0.360461
H	-2.366788	3.558202	-1.082699	C	2.439280	2.108380	2.038358
H	-3.641740	4.425055	-0.197338	H	2.686769	1.046199	2.180995
H	-4.142160	2.433927	1.153201	H	3.136919	2.688335	2.657635
H	-3.836582	1.702025	-0.444745	H	1.428038	2.268877	2.425445
C	-0.143747	-2.714545	0.057826	H	2.251037	3.554831	0.471870
C	-1.356364	-3.663875	0.224260	C	0.005809	1.511935	-2.068766
H	-2.271387	-3.177005	-0.136933	H	-0.782855	1.221392	-1.363461
H	-1.215209	-4.591721	-0.346702	H	-0.470290	2.040448	-2.905346
H	-1.517377	-3.948244	1.269502	H	0.462333	0.596602	-2.467610
C	0.017867	-2.389268	-1.435065	C	2.029340	2.920105	-2.462082
H	0.947605	-1.844082	-1.626586	H	2.596913	2.098118	-2.919564
H	0.036108	-3.303304	-2.042417	H	1.477023	3.439230	-3.259284
H	-0.814385	-1.769442	-1.795295	H	2.745843	3.634980	-2.046605
H	0.744980	-3.317755	0.333735	H	0.524436	3.298516	-1.013325
C	-0.153013	-1.739722	2.291049				

Note: Basis Set Superposition Errors

Basis set superposition errors (BSSE) arise from the inconsistent basis set treatment of molecular fragments at varying proximity (e.g. A-B versus A—B). At shorter intermolecular distances (A-B) fragments *A* and *B* access additional functions from its neighboring fragment (*B* and *A*), but at large intermolecular distances (A—B) the fragments are too far away for its basis set functions to provide stabilization (a result of insufficient overlap integrals). Only in the limit of a complete basis set (CBS), the BSSE would be reduced to zero.

Because CBS is computationally prohibitive in our case, we attempted to correct for BSSE using the counterpoise method by Boyes. This lead to relative energies that were much reduced. The longer the intermolecular distance between A and B, the more the energy was corrected by the BSSE correction. With this approach, however, one can only compare geometries if the selected fragments are identical. This prohibits a comprehensive energy correction for all structures in scheme 2. However, it does serve as a useful check for the extent of BSSE for selected geometries.

Alternatively, single-point energies were computed at the B3LYP level of theory using the aug-pVDZ basis set that is commonly used to reduce basis set superposition errors—a large increase in basis set at the MP2 level of theory was not possible due to the molecular size. Indeed, the relative energies of like aggregates was reduced. A comparison in energies between unlike aggregates using B3LYP, however, has consistently led to large energy errors as evident from B3LYP-derived relative energies of THF-solvated LDA monomers. For a consistent calculation of energies we were therefore restricted to the method of MP2/6-31G(d) and spot-checked for BSSE where possible with the counterpoise correction.

It is worth noting that not only energies but geometries as well are affected by BSSE. Transition structures **17**-**19** needed to be optimized with an additional diffuse function (6-31+G(d)) for successful convergence. Transition state optimization with counterpoise correction also led to convergence but with an O-Li distance 0.2-0.3 Å shorter on average. Even though this geometry is likely to be superior to the BSSE-uncorrected geometry, we could not include it in the comprehensive scheme because the resulting energies would not be comparable to those that were not corrected during optimization.

We therefore conclude that basis set errors need serious consideration in energy calculations as well as geometry optimizations but often cannot be comprehensively corrected. In addition we would like to caution that an increase in basis set is not always beneficial and that lower basis sets are adequate as long as one acknowledges its limitations and conducts qualitative checks for its deficiencies. In our experience a judicious level of theory is more important and meaningful for an effective computational outcome.

References

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