

A predictive chemistry DFT study of the N2O functionalization for the preparation of triazolopyridine and triazoloquinoline scaffolds

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Table S2. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness and electrophilicity of species **B** of the different predicted scaffolds at the B3LYP-D3(SMD)/Def2TZVP level of theory in tetrahydrofuran.

Table S3. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness and electrophilicity of species **B** of the different predicted scaffolds at the B3LYP-D3(SMD)/Def2SVP level of theory in tetrahydrofuran involving two explicit molecules of THF.

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Figure S1. Yield (%) vs ΔG^\ddagger (kcal/mol) plot of entries 1 to 5 of Table 1.

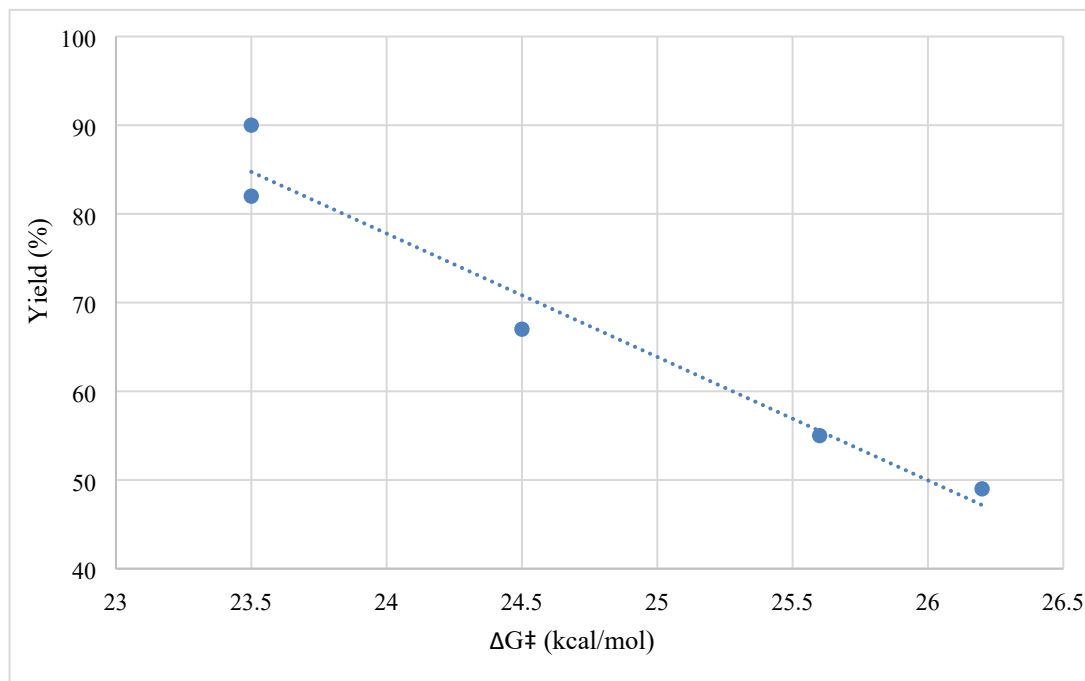
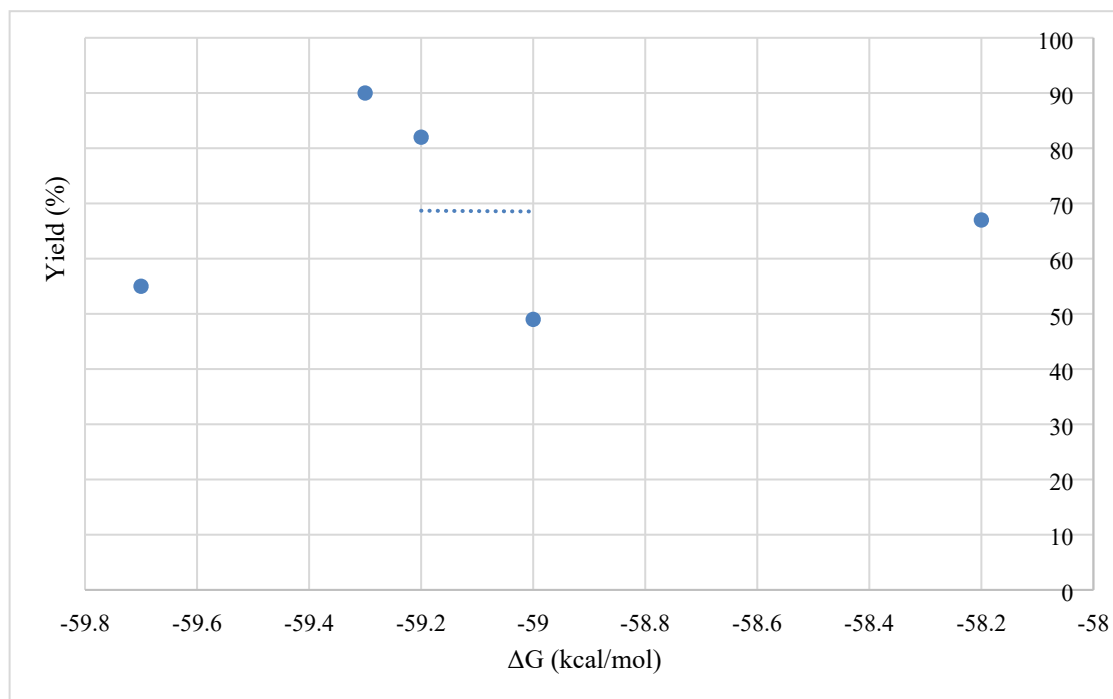


Figure S2. Yield (%) vs ΔG (kcal/mol) plot of entries 1 to 5 of Table 1.



One thing that needs to be noticed is that different scaffolds (*i.e.* triazolopyridines and triazoloquinolines) show the same trend but the regression equation is not exactly the same due to the differences in structure. Only entries 1 to 5 should be taken to study the correlation since they are substituted in the phenyl ring of the 2-benzylpyridine species. Taking those, the correlation equation shown in Figure S1 is obtained. Moreover, a clear tendency is observed in Table 1 in which it is shown that the lower the barrier of the rds, the higher the yield, so we consider that being able to obtain energy barriers for the 2 and 3-nitrogen derivatives lower than the experimental species is a clear indicative of a higher expected experimental yield for their synthesis. Considering other descriptors such as the ΔG of formation of the triazolopyridine and triazoloquinoline scaffolds, no correlation can be observed between this magnitude and the reported experimental yields. Not even considering the similar scaffolds (*i.e.* phenyl-substituted 2-benzylpyridine species) a good correlation is observed as shown in Figure S2. Therefore, that indicates that the best-found descriptor to predict the experimental yield is the ΔG^\ddagger value.

Table S1. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness and electrophilicity of species **B** of the different predicted scaffolds at the B3LYP-D3(SMD)/Def2SVP level of theory in tetrahydrofuran.

		ΔG^\ddagger (kcal/mol)	HOMO (a.u.)	LUMO (a.u.)	Chemical Potential	Chemical Hardness	Electrophilicity
Pyridine		26.7	-0.19984	-0.04667	-0.123	0.153	0.050
2N	1	24.2	-0.18909	-0.06744	-0.128	0.122	0.068
	2	24.5	-0.17917	-0.06750	-0.123	0.112	0.068
	3	22.6	-0.17840	-0.05937	-0.119	0.119	0.059
	4	22.3	-0.18005	-0.05647	-0.118	0.124	0.057
3N	5	18.3	-0.18238	-0.07009	-0.126	0.112	0.071
	6	20.6	-0.18327	-0.08375	-0.134	0.100	0.090
	7	20.7	-0.18153	-0.08996	-0.136	0.092	0.101
	8	22.2	-0.18319	-0.08976	-0.136	0.093	0.100
	9	19.1	-0.18462	-0.08614	-0.135	0.098	0.093

Table S2. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness and electrophilicity of species **B** of the different predicted scaffolds at the B3LYP-D3(SMD)/Def2TZVP level of theory in tetrahydrofuran.

		ΔG^\ddagger (kcal/mol)	HOMO (a.u.)	LUMO (a.u.)	Chemical Potential	Chemical Hardness	Electrophilicity
Pyridine		26.7	-0.21208	-0.05102	-0.132	0.161	0.054
2N	1	24.2	-0.19302	-0.07226	-0.133	0.121	0.073
	2	24.5	-0.19242	-0.07135	-0.132	0.121	0.072
	3	22.6	-0.19237	-0.0635	-0.128	0.129	0.064
	4	22.3	-0.19328	-0.06056	-0.127	0.133	0.061
3N	5	18.3	-0.19620	-0.07327	-0.135	0.123	0.074
	6	20.6	-0.19629	-0.08711	-0.142	0.109	0.092
	7	20.7	-0.19531	-0.09390	-0.145	0.101	0.103
	8	22.2	-0.19616	-0.09382	-0.145	0.102	0.103
	9	19.1	-0.19755	-0.0905	-0.144	0.107	0.097

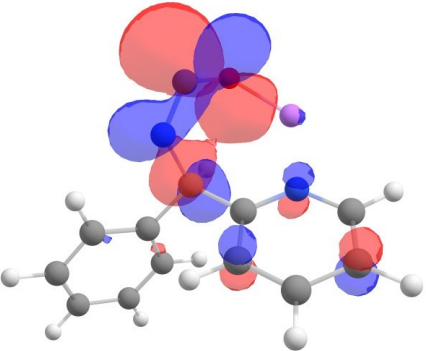
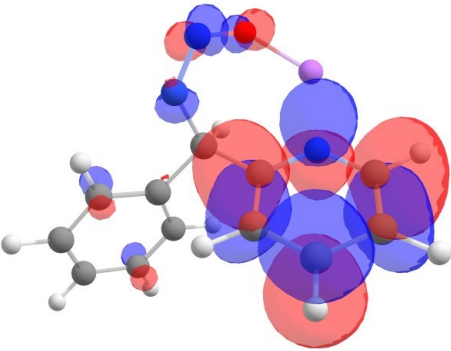
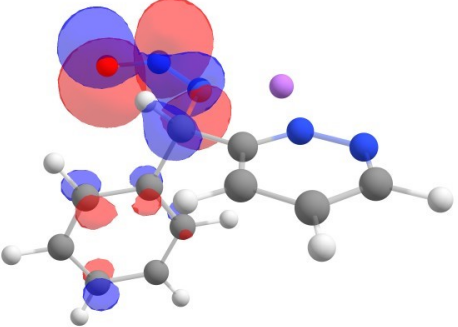
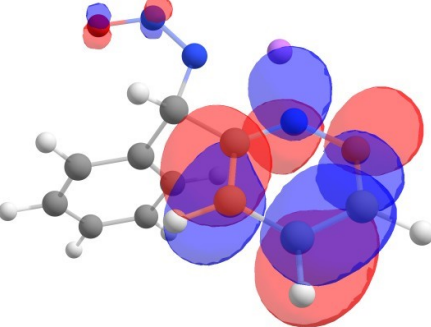
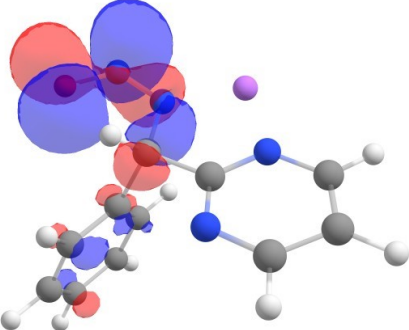
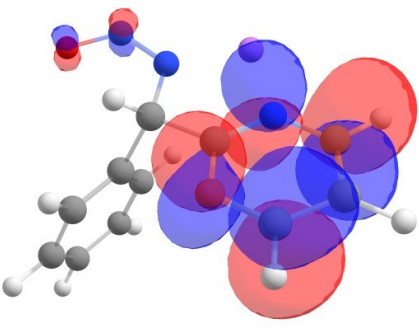
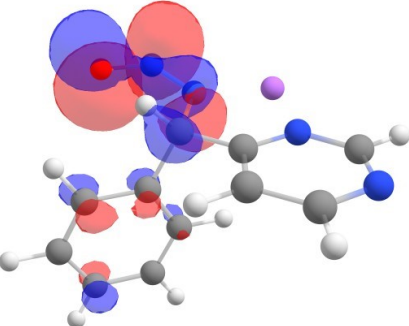
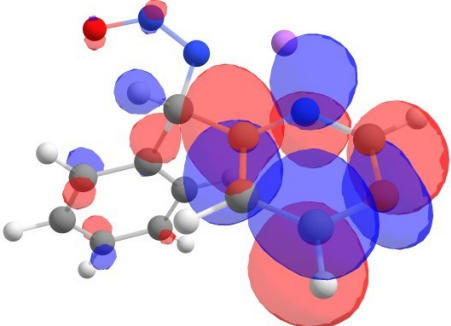
Table S3. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness and electrophilicity of species **B** of the different predicted scaffolds at the B3LYP-D3(SMD)/Def2SVP level of theory in tetrahydrofuran involving two explicit molecules of THF.

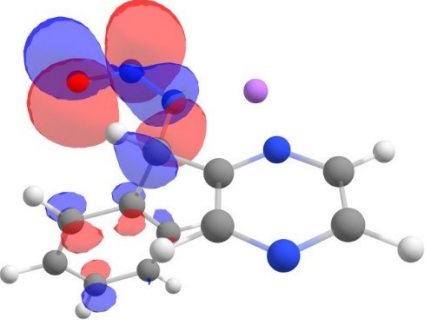
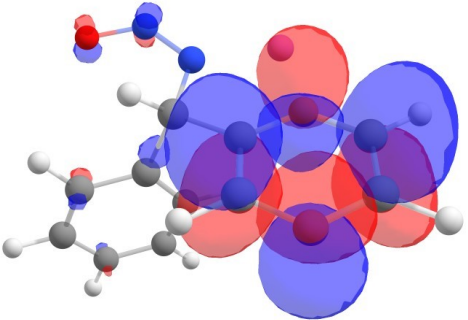
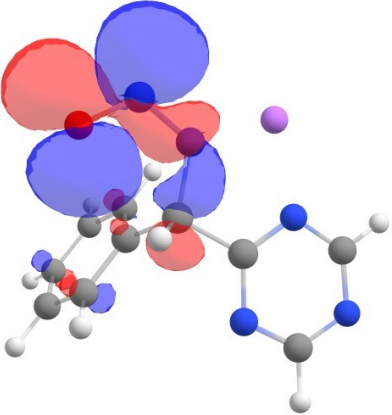
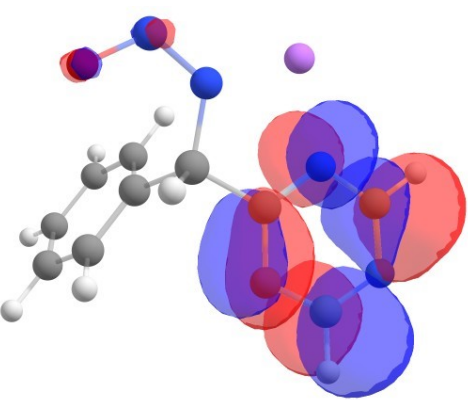
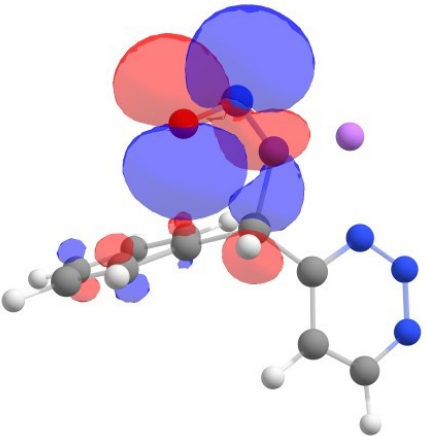
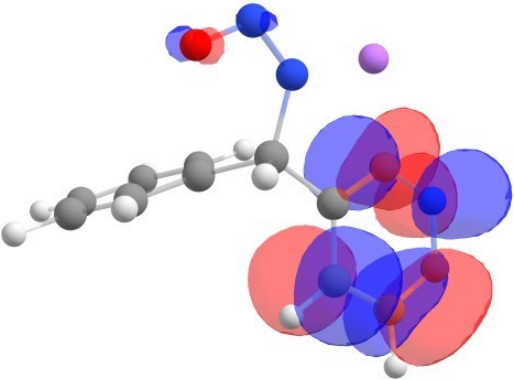
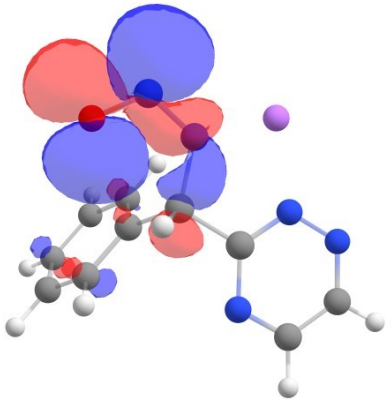
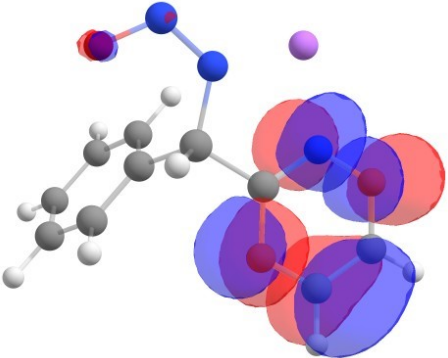
		ΔG^\ddagger (kcal/mol)	HOMO (a.u.)	LUMO (a.u.)	Chemical Potential	Chemical Hardness	Electrophilicity
Pyridine		23.5	-0.18901	-0.03924	-0.114	0.150	0.043
2N	1	21.9	-0.17251	-0.06141	-0.117	0.111	0.062
	2	21.6	-0.17210	-0.06219	-0.117	0.110	0.062
	3	21.2	-0.17013	-0.05226	-0.111	0.118	0.052
	4	18.9	-0.17201	-0.04951	-0.111	0.123	0.050
3N	5	17.0	-0.17463	-0.06277	-0.119	0.112	0.063
	6	18.2	-0.17384	-0.07759	-0.126	0.096	0.082
	7	19.8	-0.17260	-0.08497	-0.129	0.088	0.095
	8	19.8	-0.17612	-0.08289	-0.130	0.093	0.090
	9	16.1	-0.17670	-0.07917	-0.128	0.098	0.084

Table S4. Summary of the activation energy (in kcal/mol), HOMO and LUMO energies (in a.u.), chemical potential, chemical hardness and electrophilicity of species **B** of the different predicted scaffolds at the B3LYP-D3(SMD)/Def2TZVP level of theory in tetrahydrofuran including two explicit molecules of THF.

		ΔG^\ddagger (kcal/mol)	HOMO (a.u.)	LUMO (a.u.)	Chemical Potential	Chemical Hardness	Electrophilicity
Pyridine		23.5	-0.20034	-0.04205	-0.121	0.158	0.046
2N	1	21.9	-0.18429	-0.06649	-0.125	0.118	0.067
	2	21.6	-0.18410	-0.06542	-0.125	0.119	0.066
	3	21.2	-0.18213	-0.05677	-0.119	0.125	0.057
	4	18.9	-0.18373	-0.05400	-0.119	0.130	0.054
3N	5	17.0	-0.18696	-0.06624	-0.127	0.121	0.066
	6	18.2	-0.18707	-0.08044	-0.134	0.107	0.084
	7	19.8	-0.18556	-0.08820	-0.137	0.097	0.096
	8	19.8	-0.18765	-0.08652	-0.137	0.101	0.093
	9	16.1	-0.18831	-0.08372	-0.136	0.105	0.088

Table S5. HOMO and LUMO shapes of species **B** of the different predicted scaffolds at the B3LYP-D3(SMD)/Def2SVP level of theory in tetrahydrofuran.

		HOMO	LUMO
Pyridine			
2N	1		
	2		
	3		

	4		
	5		
3N	6		
	7		

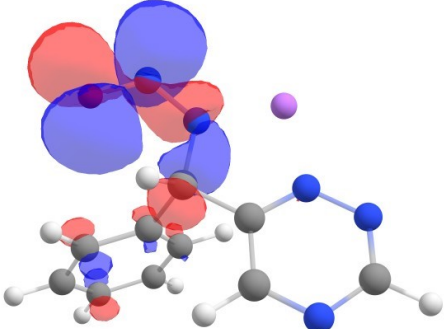
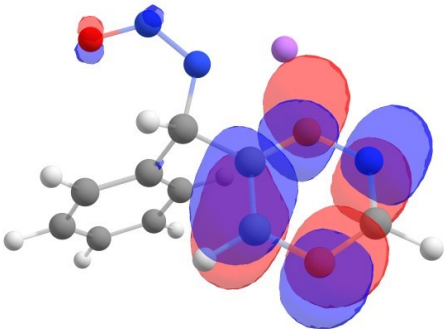
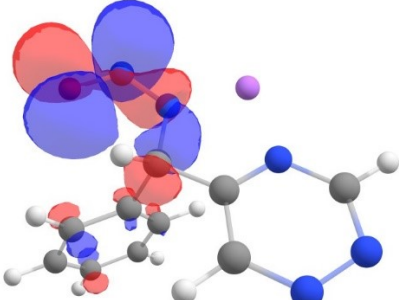
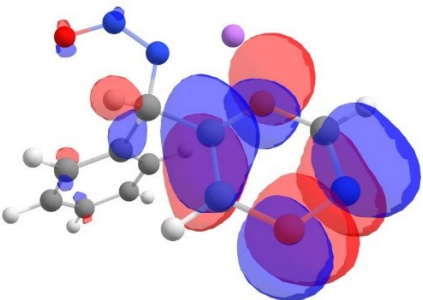
8		
9		

Table S6. B3LYP-D3(SMD)/Def2SVP Cartesian coordinates of the optimized geometries in tetrahydrofuran of the species calculated in this study.

3			
N2O SCF Done: -184.741556793 A.U.			
N	-0.000000	0.070274	-0.000000
N	0.001250	1.199698	-0.000000
O	-0.001093	-1.111226	0.000000
14			
<i>n</i> -BuLi SCF Done: -165.429354193 A.U.			
C	2.178276	-0.271361	0.000032
H	2.256985	-0.922316	-0.888681
H	2.256894	-0.922361	0.888722
H	3.057701	0.395249	0.000094
C	0.862531	0.509668	-0.000025
H	0.827533	1.177568	0.881777
H	0.827583	1.177558	-0.881837
C	-0.396946	-0.376064	-0.000047
H	-0.328128	-1.052656	0.877800
H	-0.328159	-1.052567	-0.877965
C	-1.750764	0.360746	0.000023
H	-1.753077	1.056506	-0.872754
H	-1.753029	1.056441	0.872852
Li	-3.474294	-0.750451	0.000030
13			
THF SCF Done: -232.550535764 A.U.			
C	1.180676	-0.463699	-0.000000
O	0.000007	-1.253377	-0.000001
C	-1.180670	-0.463707	-0.000000
C	-0.773022	1.024635	0.000001
C	0.773013	1.024640	0.000000
H	1.787896	-0.717991	0.889304
H	1.787896	-0.717990	-0.889304
H	-1.787896	-0.718011	-0.889298
H	-1.787897	-0.718012	0.889296
H	-1.173283	1.541944	-0.884494
H	-1.173283	1.541943	0.884496
H	1.173267	1.541957	-0.884494
H	1.173267	1.541956	0.884495
24			
A0 SCF Done: -518.876154486 A.U.			
C	-3.042623	0.929284	-0.908120
C	-1.912948	1.276794	-0.166283
C	-1.279956	0.296432	0.614863
C	-2.811156	-1.294537	-0.046215
C	-3.506514	-0.387523	-0.850829
H	-3.553771	1.675641	-1.522285
H	-1.518818	2.295596	-0.188358
H	-3.147350	-2.336000	0.025156
H	-4.386882	-0.707595	-1.412847
C	-0.020552	0.610114	1.399267
H	-0.000016	1.678407	1.659318
H	-0.054053	0.033326	2.336985
C	1.238386	0.249307	0.628392

C	2.092538	1.245100	0.131533
C	1.554039	-1.096579	0.373245
C	3.239313	0.907803	-0.597261
H	1.859266	2.297251	0.319645
C	2.697219	-1.435839	-0.354786
H	0.884735	-1.877483	0.743004
C	3.545761	-0.434031	-0.842529
H	3.895027	1.697945	-0.973736
H	2.928611	-2.488161	-0.542265
H	4.441442	-0.699567	-1.410637
N	-1.729892	-0.966758	0.668337
14			
<i>n</i> -BuH SCF Done: -158.530047497 A.U.			
C	1.959648	0.120058	-0.000001
H	2.755434	-0.643577	-0.000003
H	2.109231	0.756778	-0.889332
H	2.109235	0.756778	0.889328
C	0.568506	-0.513047	0.000002
H	0.461278	-1.171432	-0.882237
H	0.461280	-1.171429	0.882243
C	-0.568507	0.513047	0.000002
H	-0.461280	1.171429	0.882243
H	-0.461278	1.171431	-0.882237
C	-1.959648	-0.120058	-0.000001
H	-2.109235	-0.756777	0.889329
H	-2.755434	0.643577	-0.000004
H	-2.109230	-0.756779	-0.889331
38			
TS-A0A SCF Done: -684.310742454 A.U.			
Li	-0.729333	-2.547494	-0.797424
C	4.904664	-1.959246	0.050030
H	5.747681	-2.358844	0.638803
H	5.015245	-2.332538	-0.983291
H	5.014517	-0.861324	0.014591
C	3.552434	-2.359248	0.642179
H	3.481836	-3.461940	0.698121
H	3.483794	-2.000718	1.686249
C	2.348751	-1.818681	-0.143977
H	2.431821	-2.172721	-1.192241
H	2.446011	-0.716909	-0.208827
C	0.967335	-2.168239	0.413752
H	0.889436	-1.846894	1.471033
H	0.849334	-3.278899	0.441458
C	-4.086219	0.392695	0.576049
C	-2.787133	0.744451	0.230733
C	-1.930997	-0.215608	-0.352628
C	-3.631858	-1.822499	-0.204140
C	-4.531998	-0.919942	0.350801
H	-4.759887	1.138803	1.006885
H	-2.429636	1.763981	0.379860
H	-3.926429	-2.862309	-0.384754
H	-5.546544	-1.233072	0.604537
C	-0.537406	0.016919	-0.784418
H	0.119584	-1.018136	-0.235299
H	-0.436314	-0.203293	-1.861524
C	0.184431	1.254686	-0.410021

C	0.244508	1.693281	0.933439
C	0.928841	1.986795	-1.361214
C	0.995536	2.812166	1.299890
H	-0.297925	1.135259	1.701562
C	1.687937	3.100518	-0.993583
H	0.909866	1.668705	-2.408220
C	1.724562	3.525948	0.340038
H	1.021165	3.124394	2.348243
H	2.252558	3.644663	-1.756661
H	2.315733	4.399215	0.628319
N	-2.370597	-1.495558	-0.531167
24			
A SCF Done: -525.827147397 A.U.			
C	2.812745	1.527791	0.388269
C	1.517823	1.050237	0.332805
C	1.276660	-0.338554	0.066287
C	3.612376	-0.661625	-0.139258
C	3.905798	0.662629	0.158141
H	2.989739	2.580338	0.630342
H	0.679876	1.710622	0.554006
H	4.418367	-1.372818	-0.357792
H	4.938322	1.013512	0.199876
C	0.006995	-0.993712	0.040856
H	0.040746	-2.045957	0.363470
C	-1.322510	-0.410711	0.016511
C	-2.430397	-1.164644	0.495704
C	-1.626602	0.873757	-0.513093
C	-3.732692	-0.669315	0.464486
H	-2.247844	-2.163466	0.905366
C	-2.932144	1.368583	-0.535047
H	-0.829755	1.482722	-0.944215
C	-4.001862	0.609300	-0.044525
H	-4.550518	-1.287063	0.848760
H	-3.117180	2.362633	-0.954468
H	-5.022105	1.001078	-0.063719
N	2.365953	-1.151685	-0.203347
Li	1.207176	-2.114075	-1.381674
27			
TS-AB SCF Done: -710.566661346 A.U.			
C	-1.087275	-0.482041	0.343649
C	-1.141932	-1.814030	-0.188312
C	-2.352003	-2.455771	-0.361236
C	-3.556168	-1.803594	-0.020217
C	-3.447304	-0.519686	0.497443
N	-2.285866	0.131481	0.674564
H	-2.370842	-3.478148	-0.750788
H	-0.215577	-2.338523	-0.415760
H	-4.530781	-2.277715	-0.146076
H	-4.352538	0.030720	0.785245
C	0.104742	0.247279	0.600706
H	-0.018350	1.075448	1.309438
N	-0.047704	1.841232	-1.401686
N	-0.750526	2.649940	-1.009830
O	-1.486556	3.196669	-0.193306
C	1.488746	-0.108029	0.343393
C	2.505172	0.431863	1.178644

C	1.931361	-0.915393	-0.739117
C	3.856163	0.159560	0.970277
H	2.211896	1.075535	2.014139
C	3.284898	-1.191505	-0.939983
H	1.207426	-1.297134	-1.460370
C	4.263590	-0.665572	-0.087164
H	4.601859	0.593113	1.643879
H	3.580943	-1.815743	-1.788857
H	5.322243	-0.884006	-0.249689
Li	-2.351701	2.028682	1.058483
27			
TS-AB1 SCF Done: -710.572093865 A.U.			
C	-1.261142	-0.344339	0.413993
C	-1.428542	-1.580945	-0.284346
C	-2.695691	-2.055767	-0.570342
C	-3.831204	-1.318368	-0.180521
C	-3.608812	-0.123693	0.493736
N	-2.390207	0.358510	0.780901
H	-2.811591	-3.013306	-1.086722
H	-0.553196	-2.171486	-0.551348
H	-4.845395	-1.663109	-0.388867
H	-4.457328	0.490886	0.818178
C	-0.006759	0.222707	0.804579
H	-0.066893	0.890138	1.673662
N	0.037587	2.137399	-0.837640
N	0.859437	1.953111	-1.609052
O	-0.861297	2.836671	-0.353233
C	1.330560	-0.220380	0.484414
C	1.689696	-0.820016	-0.752170
C	2.394142	0.046542	1.390653
C	3.012040	-1.177310	-1.032959
H	0.927590	-0.988499	-1.513442
C	3.709901	-0.304000	1.103437
H	2.162924	0.532632	2.343717
C	4.032929	-0.931436	-0.110487
H	3.246349	-1.642441	-1.995301
H	4.496302	-0.091214	1.833920
H	5.065614	-1.211928	-0.333774
Li	-1.948145	2.224619	1.042158
27			
TS-AB2 SCF Done: -710.538731956 A.U.			
C	0.783185	0.496773	-0.009337
C	0.705876	1.928714	0.224570
C	1.834438	2.694177	0.324147
C	3.130675	2.104037	0.196480
C	3.192020	0.749898	0.009597
N	2.083017	-0.043603	-0.029056
H	1.742676	3.769852	0.498241
H	-0.274022	2.388754	0.329987
H	4.042502	2.699258	0.258216
H	4.142067	0.218665	-0.098185
N	2.461471	-1.483259	-1.149967
N	2.285721	-2.493951	-0.543572
O	1.857837	-2.726305	0.619243
C	-0.289665	-0.389226	-0.084716
C	-1.732229	-0.139113	-0.068614

C	-2.584280	-1.199538	0.334082
C	-2.361945	1.061317	-0.476556
C	-3.970602	-1.058633	0.364171
H	-2.134558	-2.151021	0.634514
C	-3.752310	1.201902	-0.441572
H	-1.765982	1.885376	-0.869542
C	-4.569389	0.150401	-0.014381
H	-4.591076	-1.899692	0.687149
H	-4.201477	2.144248	-0.768752
H	-5.656123	0.265058	0.011081
H	-0.038577	-1.438887	-0.266343
Li	1.248593	-1.176580	1.513541
27			
B SCF Done: -710.610038845 A.U.			
C	-1.798923	-2.341085	-1.011814
C	-0.821667	-1.359711	-0.860426
C	-1.043791	-0.294125	0.025616
C	-3.136666	-1.146104	0.572094
C	-2.982150	-2.241927	-0.273375
H	-1.638426	-3.177666	-1.696741
H	0.116252	-1.414235	-1.414620
H	-4.053893	-1.020829	1.157055
H	-3.772138	-2.991251	-0.353385
C	-0.010823	0.816058	0.197782
H	-0.183209	1.271269	1.188154
C	1.414793	0.279763	0.171891
C	2.279164	0.491404	-0.911198
C	1.875939	-0.468946	1.267926
C	3.575128	-0.038843	-0.899811
H	1.926433	1.080079	-1.758704
C	3.168189	-0.999117	1.280659
H	1.210806	-0.638770	2.120264
C	4.024200	-0.786000	0.193006
H	4.237559	0.135861	-1.752344
H	3.510601	-1.577340	2.143376
H	5.037006	-1.197935	0.200870
N	-2.200068	-0.193084	0.715786
N	-1.033184	2.760555	-0.682338
N	-0.199496	1.831407	-0.867639
O	-1.735591	2.798137	0.412095
Li	-2.579130	1.628457	1.398185
40			
B-THF SCF Done: -943.194534791 A.U.			
C	1.709397	3.281337	-1.118799
C	1.735149	2.081793	-0.410135
C	0.524669	1.467053	-0.055146
C	-0.682216	3.176504	-1.060842
C	0.474782	3.842485	-1.460570
H	2.642594	3.773576	-1.404796
H	2.680842	1.612356	-0.135038
H	-1.670300	3.584660	-1.298373
H	0.406757	4.777093	-2.020912
C	0.500117	0.177426	0.757618
H	-0.489142	-0.282658	0.607895
C	1.543566	-0.823049	0.283621
C	2.720148	-1.081624	1.000078

C	1.322665	-1.507536	-0.923931
C	3.658576	-2.000926	0.515557
H	2.885844	-0.560390	1.943637
C	2.257755	-2.425409	-1.408615
H	0.406085	-1.314600	-1.489419
C	3.432602	-2.674808	-0.688534
H	4.571880	-2.192333	1.086007
H	2.068016	-2.950847	-2.348689
H	4.165685	-3.393943	-1.063941
N	-0.661995	2.024253	-0.372629
N	-0.307673	0.832248	2.879652
N	0.701448	0.507478	2.190212
O	-1.481587	0.891503	2.328912
Li	-2.159192	1.202754	0.697395
C	-3.183265	-1.465647	0.699796
O	-3.000762	-0.287756	-0.119742
C	-2.719402	-0.671254	-1.487847
C	-2.737226	-2.203523	-1.508084
C	-2.442790	-2.566733	-0.046245
H	-2.780122	-1.241259	1.698171
H	-4.262979	-1.686583	0.784292
H	-3.476464	-0.221772	-2.150402
H	-1.733020	-0.260778	-1.760753
H	-3.734190	-2.572769	-1.797756
H	-2.002938	-2.615774	-2.215706
H	-2.790067	-3.572475	0.231914
H	-1.361741	-2.504125	0.160143

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B-THF2 SCF Done: -1175.77377089 A.U.

C	-1.468024	-3.620503	-1.288257
C	-1.879696	-2.573335	-0.465939
C	-1.005023	-1.500899	-0.229730
C	0.620325	-2.481405	-1.563011
C	-0.190768	-3.576569	-1.856854
H	-2.136247	-4.462966	-1.485399
H	-2.871082	-2.574010	-0.010108
H	1.633839	-2.409577	-1.971895
H	0.172595	-4.373534	-2.508949
C	-1.383688	-0.357661	0.703866
H	-0.716129	0.482913	0.463110
C	-2.817645	0.107323	0.496999
C	-3.848513	-0.213592	1.391402
C	-3.125587	0.877151	-0.638074
C	-5.158070	0.220626	1.153087
H	-3.607724	-0.800204	2.278632
C	-4.431673	1.311984	-0.877572
H	-2.329803	1.136996	-1.341803
C	-5.455399	0.983250	0.019393
H	-5.950753	-0.038391	1.860786
H	-4.651155	1.912437	-1.764833
H	-6.478282	1.323415	-0.163859
N	0.227597	-1.472325	-0.772073
N	-0.020814	-0.667571	2.610439
N	-1.175464	-0.794168	2.107432
O	0.953678	-0.194974	1.900469
Li	1.504382	-0.162025	0.137940
C	1.100540	2.713208	0.336257

O	1.291215	1.632371	-0.598036
C	0.618405	1.920162	-1.841752
C	-0.062228	3.282225	-1.652242
C	-0.179538	3.397811	-0.125663
H	1.044463	2.274267	1.343086
H	1.967554	3.398490	0.286831
H	1.356353	1.920424	-2.661018
H	-0.104502	1.110105	-2.033315
H	0.576926	4.088850	-2.046063
H	-1.032468	3.336074	-2.167739
H	-0.255243	4.436639	0.227711
H	-1.059327	2.844033	0.239824
C	4.065022	-0.869519	1.234159
O	3.379236	-0.582932	-0.004589
C	4.245518	0.150723	-0.898355
C	5.597730	0.245520	-0.186348
C	5.196294	0.148994	1.291402
H	3.328847	-0.783695	2.046633
H	4.455096	-1.904040	1.203847
H	4.299496	-0.380158	-1.863131
H	3.796274	1.143155	-1.071095
H	6.239091	-0.608168	-0.460743
H	6.136361	1.171242	-0.437411
H	6.018722	-0.166801	1.950229
H	4.813794	1.118346	1.652907

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B1 SCF Done: -710.576631467 A.U.

C	1.204964	-0.234988	-0.224727
C	1.100324	-1.565758	0.212854
C	2.251930	-2.338025	0.363725
C	3.496343	-1.774251	0.076501
C	3.523074	-0.449482	-0.356330
N	2.420051	0.297250	-0.506277
H	2.173577	-3.375218	0.699676
H	0.123813	-2.000191	0.419480
H	4.423527	-2.341230	0.178537
H	4.475888	0.034895	-0.596224
C	0.007259	0.662163	-0.440763
H	0.094802	1.113831	-1.435630
N	0.161930	1.975039	0.541492
N	-0.383679	2.105780	1.585775
O	0.995332	2.827865	-0.074573
C	-1.354868	0.066179	-0.276842
C	-1.805186	-0.434151	0.959771
C	-2.238908	0.050323	-1.369070
C	-3.099999	-0.945393	1.089611
H	-1.139019	-0.415610	1.821627
C	-3.531957	-0.464998	-1.241073
H	-1.906836	0.447888	-2.332655
C	-3.966613	-0.964785	-0.008685
H	-3.434220	-1.331202	2.056674
H	-4.202082	-0.472678	-2.105017
H	-4.977911	-1.367324	0.095855
Li	2.499840	2.265475	-0.754166

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B1-THF2 SCF Done: -1175.73952460 A.U.

C	0.864368	-1.306535	0.635032
C	1.575390	-2.389362	1.184349
C	0.900135	-3.328568	1.963368
C	-0.472228	-3.181090	2.183136
C	-1.105849	-2.078730	1.607314
N	-0.462619	-1.172100	0.866213
H	1.445613	-4.170484	2.398072
H	2.646731	-2.488391	1.016870
H	-1.037448	-3.894731	2.785942
H	-2.180034	-1.912508	1.745083
C	1.467429	-0.244245	-0.231449
H	0.978013	0.706889	-0.000890
N	0.886215	-0.536243	-1.817103
N	1.523543	-1.080735	-2.653172
O	-0.339282	-0.048319	-1.862323
C	2.945045	-0.068422	-0.267188
C	3.814349	-1.066736	-0.748983
C	3.500082	1.161346	0.134073
C	5.193834	-0.841226	-0.808070
H	3.405607	-2.015433	-1.093006
C	4.877789	1.384838	0.080504
H	2.836632	1.951801	0.496710
C	5.731579	0.380788	-0.391792
H	5.853229	-1.628285	-1.184647
H	5.285779	2.346047	0.405148
H	6.810712	0.551692	-0.436586
Li	-1.414882	0.142094	-0.375119
C	-1.022214	2.260819	1.717815
O	-1.281545	1.932798	0.338994
C	-0.848129	3.001529	-0.529189
C	0.039250	3.884926	0.341574
C	-0.624186	3.736161	1.716940
H	-1.925998	2.047684	2.310823
H	-0.204727	1.618297	2.090873
H	-0.334941	2.548442	-1.390621
H	-1.736147	3.551331	-0.891397
H	1.067086	3.486630	0.365573
H	0.081928	4.923622	-0.017313
H	0.038895	3.991004	2.556741
H	-1.520242	4.375771	1.779110
C	-4.330784	0.614089	-0.067072
O	-3.272732	-0.316206	-0.377523
C	-3.801428	-1.486863	-1.035191
C	-5.225103	-1.110627	-1.435492
C	-5.626504	-0.158987	-0.301357
H	-4.204339	0.962516	0.969785
H	-4.250566	1.487013	-0.739027
H	-3.149558	-1.736387	-1.886383
H	-3.788909	-2.333729	-0.325344
H	-5.222138	-0.577188	-2.400427
H	-5.881491	-1.988287	-1.527960
H	-6.468097	0.501552	-0.556691
H	-5.899404	-0.732420	0.600241
27			
B2 SCF Done: -710.550072599 A.U.			
C	0.824951	0.353726	-0.138452
C	0.821870	1.692710	0.412325

C	1.962192	2.443972	0.519698
C	3.215395	1.923294	0.089103
C	3.237300	0.634698	-0.370836
N	2.111322	-0.127117	-0.442876
H	1.906184	3.449173	0.945678
H	-0.124592	2.092387	0.769952
H	4.135617	2.505284	0.138544
H	4.146199	0.125058	-0.695745
N	2.333744	-1.450415	-0.997647
N	2.185200	-2.412214	-0.186525
O	1.813841	-2.205087	1.019328
C	-0.287033	-0.473310	-0.298848
C	-1.713420	-0.146901	-0.185463
C	-2.622803	-1.216265	0.026035
C	-2.275817	1.145597	-0.321503
C	-3.996624	-1.004635	0.131819
H	-2.229272	-2.234534	0.107568
C	-3.653278	1.355561	-0.210603
H	-1.637703	1.996914	-0.560013
C	-4.525868	0.288278	0.025221
H	-4.661753	-1.856848	0.298828
H	-4.048992	2.368836	-0.326647
H	-5.602252	0.457888	0.110672
H	-0.092220	-1.474923	-0.690843
Li	0.455006	-1.280221	1.688580

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TS-BC SCF Done: -710.563522065 A.U.

C	1.316261	-0.055793	0.092048
C	1.659526	-1.132436	0.949391
C	2.926641	-1.692369	0.889407
C	3.870790	-1.176670	-0.014592
C	3.478463	-0.110035	-0.813104
N	2.248640	0.432227	-0.776405
H	3.192090	-2.517188	1.556535
H	0.928519	-1.491988	1.674881
H	4.881224	-1.583145	-0.086288
H	4.181259	0.334627	-1.526654
C	0.004952	0.603183	0.151398
H	-0.359897	1.494091	1.322753
Li	1.465439	1.866739	-1.884373
N	0.027165	1.884187	-0.583289
N	-0.341018	2.879905	0.106701
O	-0.703065	2.589991	1.336863
C	-1.258642	-0.168981	-0.001414
C	-1.296355	-1.579386	-0.124167
C	-2.507999	0.501398	-0.057520
C	-2.501145	-2.273078	-0.260077
H	-0.368032	-2.151510	-0.132871
C	-3.708674	-0.195885	-0.200671
H	-2.546604	1.588576	0.019295
C	-3.722592	-1.592041	-0.295290
H	-2.479049	-3.363219	-0.352534
H	-4.647834	0.364421	-0.236068
H	-4.664336	-2.136488	-0.402352

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TS-BC-THF SCF Done: -943.147983944 A.U.

C	0.941861	1.412637	0.321675
C	1.929949	2.393100	0.599213
C	1.645039	3.737917	0.418421
C	0.368919	4.123075	-0.026887
C	-0.558432	3.115345	-0.261579
N	-0.291547	1.807766	-0.104932
H	2.405141	4.492329	0.640040
H	2.901183	2.079845	0.984795
H	0.102218	5.171377	-0.173362
H	-1.571920	3.362802	-0.597767
C	1.175634	-0.018653	0.548981
H	1.205991	-0.564748	1.959046
Li	-1.479482	0.245936	-0.477309
N	-0.089642	-0.776667	0.471959
N	-0.337872	-1.464205	1.503601
O	0.582579	-1.403639	2.443513
C	2.342529	-0.721941	-0.050661
C	3.326559	-0.069156	-0.832489
C	2.500344	-2.121998	0.118757
C	4.410192	-0.761695	-1.378141
H	3.239642	0.998275	-1.038352
C	3.580566	-2.810917	-0.434903
H	1.770814	-2.684117	0.702961
C	4.554330	-2.139386	-1.183065
H	5.144553	-0.213485	-1.976228
H	3.661748	-3.890251	-0.274427
H	5.402340	-2.679766	-1.611667
C	-4.260871	-0.144943	-1.529447
O	-3.295177	-0.193216	-0.449606
C	-3.844467	-0.909133	0.687185
C	-5.031923	-1.677424	0.123205
C	-5.554683	-0.705000	-0.941647
H	-4.350767	0.895413	-1.879836
H	-3.887310	-0.767082	-2.361431
H	-3.051440	-1.541868	1.112711
H	-4.160925	-0.175610	1.450159
H	-4.692383	-2.616837	-0.343480
H	-5.775163	-1.922747	0.895741
H	-6.182950	-1.185106	-1.705907
H	-6.141403	0.099382	-0.468428

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TS-BC-THF2 SCF Done: -1175.73272690 A.U.

C	1.179538	1.842013	0.322786
C	2.339998	2.630929	0.120595
C	2.263767	3.798263	-0.626453
C	1.028685	4.196410	-1.162926
C	-0.072223	3.382945	-0.912556
N	-0.007490	2.243592	-0.208173
H	3.157234	4.410520	-0.778308
H	3.281317	2.325701	0.580629
H	0.923569	5.112753	-1.746921
H	-1.060052	3.651246	-1.305052
C	1.199946	0.617121	1.137308
H	1.353790	0.706300	2.636055
Li	-1.340655	0.701505	-0.058835
N	-0.174253	0.190040	1.480279

N	-0.374251	0.067286	2.718673
O	0.675001	0.315340	3.481015
C	2.101911	-0.511900	0.798061
C	3.063701	-0.459453	-0.240956
C	1.999532	-1.742346	1.498155
C	3.872259	-1.555646	-0.550151
H	3.170784	0.446579	-0.838226
C	2.805995	-2.836614	1.182120
H	1.275736	-1.844884	2.307844
C	3.754912	-2.758253	0.155758
H	4.595518	-1.468725	-1.366750
H	2.688457	-3.765527	1.748315
H	4.385533	-3.616248	-0.090718
C	-4.090833	0.191827	-0.874380
O	-3.229706	0.602139	0.213941
C	-3.743236	0.079083	1.454744
C	-4.422634	-1.221239	1.050295
C	-5.082021	-0.823730	-0.279311
H	-4.596182	1.078413	-1.292817
H	-3.448127	-0.244391	-1.654952
H	-2.900868	-0.038643	2.151107
H	-4.467411	0.794884	1.888058
H	-3.662168	-2.003988	0.893027
H	-5.140569	-1.580264	1.802347
H	-5.251644	-1.678068	-0.950857
H	-6.055550	-0.344396	-0.089744
C	-0.966255	-1.961516	-1.109457
O	-0.925016	-0.560469	-1.460000
C	0.043906	-0.329968	-2.505294
C	0.395095	-1.714102	-3.043580
C	0.248397	-2.585840	-1.790193
H	-0.944475	-2.047988	-0.012421
H	-1.912936	-2.392366	-1.482988
H	-0.404063	0.340043	-3.255870
H	0.926689	0.168011	-2.071199
H	-0.327145	-2.022670	-3.817731
H	1.404732	-1.745399	-3.479075
H	0.100779	-3.653127	-2.011377
H	1.136102	-2.482680	-1.148361
27			
TS-B1C SCF Done: -710.520948952 A.U.			
C	-1.159796	-0.259869	0.091820
C	-0.981032	-1.654935	-0.054037
C	-2.084945	-2.474437	-0.252133
C	-3.365601	-1.907094	-0.313661
C	-3.466436	-0.528368	-0.163543
N	-2.410251	0.277072	0.039523
H	-1.948985	-3.552658	-0.372524
H	0.022851	-2.077918	-0.019760
H	-4.257822	-2.514033	-0.477373
H	-4.446062	-0.039147	-0.204852
C	-0.020355	0.645820	0.363470
H	-0.417371	1.450971	1.394548
N	-0.259168	1.995706	-0.270513
N	-0.078505	2.568382	-1.257467
O	-0.931795	2.587384	1.106698
C	1.368070	0.128376	0.171259

C	1.998748	-0.527517	1.245209
C	2.069080	0.247558	-1.043544
C	3.285089	-1.056381	1.108996
H	1.467857	-0.618501	2.196784
C	3.364635	-0.262617	-1.172566
H	1.595450	0.748161	-1.890033
C	3.976478	-0.920891	-0.100335
H	3.754842	-1.565050	1.955457
H	3.895605	-0.153230	-2.122442
H	4.987261	-1.324208	-0.205474
Li	-2.622470	2.160182	0.675227

53

TS-B1C-THF2 SCF Done: -1175.68367864 A.U.

C	-1.382650	-0.867350	0.833973
C	-2.288393	-1.574409	1.661019
C	-1.817882	-2.235694	2.788787
C	-0.451628	-2.187328	3.101198
C	0.376270	-1.465908	2.245026
N	-0.060846	-0.831487	1.148823
H	-2.515563	-2.777808	3.433337
H	-3.350313	-1.589877	1.415366
H	-0.043380	-2.686595	3.981943
H	1.451371	-1.391370	2.447158
C	-1.806386	-0.197227	-0.412009
H	-0.894510	-0.575691	-1.384003
N	-0.933922	1.015468	-0.691292
N	-0.893843	2.148995	-0.417329
O	0.045718	0.242830	-1.601628
C	-3.259203	0.016628	-0.668170
C	-4.023846	-1.052074	-1.178158
C	-3.913438	1.238573	-0.417462
C	-5.392570	-0.910449	-1.418752
H	-3.528538	-2.003717	-1.390263
C	-5.279382	1.386140	-0.679471
H	-3.340817	2.076835	-0.017098
C	-6.027657	0.313374	-1.175389
H	-5.963886	-1.756260	-1.811817
H	-5.764679	2.346675	-0.483200
H	-7.096582	0.429835	-1.373708
Li	1.307420	-0.157125	-0.242253
C	1.739557	2.138595	1.633318
O	2.256651	1.325144	0.558946
C	2.995087	2.137761	-0.378256
C	3.191437	3.482372	0.317649
C	1.920113	3.580777	1.169970
H	0.690247	1.861201	1.810538
H	2.320730	1.926215	2.549324
H	3.937973	1.623536	-0.623752
H	2.399606	2.243648	-1.302009
H	4.086600	3.455447	0.961417
H	3.306371	4.309558	-0.398238
H	2.005595	4.285571	2.010224
H	1.063689	3.877656	0.544535
C	3.069737	-1.617070	-2.128140
O	2.743750	-1.309665	-0.755641
C	3.894986	-1.495097	0.092864
C	5.080339	-1.610211	-0.861319

C	4.437794	-2.293341	-2.075092
H	2.274707	-2.253410	-2.546742
H	3.104038	-0.676761	-2.706686
H	3.956113	-0.639358	0.782386
H	3.760632	-2.419097	0.684267
H	5.448208	-0.607649	-1.136570
H	5.916661	-2.177152	-0.426794
H	5.005901	-2.161314	-3.007584
H	4.325180	-3.374409	-1.889623
27			
C SCF Done: -710.623929273 A.U.			
C	-1.763526	-2.820942	-0.298197
C	-0.683957	-1.944982	-0.358096
C	-0.919759	-0.558102	-0.276778
C	-3.207253	-0.924634	-0.108761
C	-3.058875	-2.308223	-0.171578
H	-1.594790	-3.898762	-0.364046
H	0.330135	-2.322914	-0.486577
H	-4.203494	-0.478958	-0.011628
H	-3.933322	-2.959501	-0.125219
C	0.187453	0.408412	-0.364959
C	1.617637	0.159854	-0.065944
C	2.627881	0.827497	-0.785997
C	1.993550	-0.721510	0.966966
C	3.974276	0.616156	-0.483490
H	2.357646	1.514157	-1.592690
C	3.342496	-0.939584	1.254741
H	1.227072	-1.227540	1.557235
C	4.339015	-0.272868	0.533417
H	4.743530	1.143571	-1.053669
H	3.615188	-1.627162	2.059709
H	5.393615	-0.442633	0.764717
N	-2.174526	-0.068716	-0.148836
N	-0.419858	2.660287	-1.113693
N	-0.136273	1.614775	-0.761660
Li	-2.837576	1.772504	0.380508
O	-3.409613	2.861763	1.400964
H	-3.724983	3.517254	2.024306
53			
C-THF2 SCF Done: -1175.77102150 A.U.			
C	1.618306	2.737042	2.433150
C	2.263576	1.712703	1.747468
C	1.489251	0.735430	1.087412
C	-0.468505	1.762265	1.781586
C	0.219480	2.764688	2.464140
H	2.203203	3.499074	2.954848
H	3.351954	1.648286	1.739876
H	-1.562320	1.753839	1.752406
H	-0.326844	3.544931	2.997599
C	2.127942	-0.407743	0.411887
C	3.465577	-0.433997	-0.216785
C	4.210103	-1.629231	-0.294276
C	4.014634	0.734315	-0.784280
C	5.460896	-1.652418	-0.913164
H	3.808208	-2.549694	0.137391
C	5.272288	0.707169	-1.390458

H	3.446466	1.666266	-0.765713
C	6.003325	-0.483867	-1.459547
H	6.019426	-2.591108	-0.960849
H	5.677771	1.625087	-1.824651
H	6.985360	-0.502347	-1.938882
N	0.140207	0.785067	1.095864
N	0.882093	-2.515611	0.416744
N	1.443763	-1.528344	0.407383
Li	-1.145556	-0.176939	-0.314212
O	-0.860961	-0.642317	-1.958956
H	-0.772849	-0.293001	-2.850783
C	-3.654622	0.694173	-1.234578
O	-2.635303	1.284928	-0.405504
C	-2.079509	2.347740	-1.189395
C	-3.294145	3.030397	-1.816884
C	-4.273271	1.853522	-2.046368
H	-3.150875	-0.038817	-1.888917
H	-4.370853	0.183064	-0.575850
H	-1.487284	2.997435	-0.529009
H	-1.415192	1.904623	-1.955291
H	-3.721277	3.759055	-1.109900
H	-3.035890	3.566975	-2.742122
H	-5.287389	2.103146	-1.700103
H	-4.344344	1.582516	-3.110737
C	-3.028098	-1.497426	1.647480
O	-2.004007	-1.650016	0.652791
C	-2.295256	-2.769975	-0.207862
C	-3.802904	-2.957006	-0.090290
C	-4.043312	-2.620257	1.389233
H	-2.575794	-1.553490	2.652564
H	-3.479432	-0.496559	1.532756
H	-1.923057	-2.491784	-1.207014
H	-1.753906	-3.662881	0.158057
H	-4.326011	-2.239743	-0.743333
H	-4.128262	-3.972326	-0.362871
H	-5.075635	-2.308717	1.608719
H	-3.813291	-3.496696	2.017073
27			
TS-CD SCF Done: -710.594298101 A.U.			
C	-1.628674	-0.056607	-0.080766
C	-1.936119	-1.429993	0.073028
C	-3.255301	-1.795513	0.310809
C	-4.257800	-0.815390	0.392948
C	-3.884219	0.512889	0.208747
N	-2.615984	0.853156	-0.022543
H	-3.508724	-2.852347	0.426701
H	-1.161566	-2.189849	-0.014155
H	-5.300884	-1.076425	0.580093
H	-4.615127	1.327411	0.238639
C	-0.306722	0.516727	-0.357966
N	-0.467241	1.832972	-0.539659
N	-1.376727	2.560620	-0.489891
C	1.016660	-0.091125	-0.465844
C	1.372403	-1.275063	0.223454
C	2.021701	0.545365	-1.238308
C	2.661650	-1.812538	0.115551
H	0.655692	-1.762616	0.883423

C	3.310482	0.014406	-1.327327
H	1.782968	1.469056	-1.770035
C	3.640679	-1.175144	-0.657943
H	2.907648	-2.722671	0.667711
H	4.064825	0.534777	-1.922187
H	4.649024	-1.588144	-0.727314
Li	2.952454	0.442025	1.110639
O	3.346406	1.275028	2.412722
H	3.588765	1.779189	3.189790

53

TS-CD-THF2 SCF Done: -1175.75592189 A.U.

C	-1.230532	-1.522696	-0.941874
C	0.090396	-1.479991	-1.453508
C	0.828897	-2.653591	-1.482016
C	0.272380	-3.854570	-1.003324
C	-1.035495	-3.824225	-0.530652
N	-1.742435	-2.691639	-0.517820
H	1.846203	-2.640434	-1.879788
H	0.510320	-0.545620	-1.819455
H	0.835979	-4.789174	-1.011286
H	-1.537856	-4.723512	-0.160255
C	-2.158119	-0.399996	-0.846064
N	-3.323330	-0.875836	-0.398832
N	-3.676628	-1.946910	-0.071290
C	-1.938104	1.030138	-1.084214
C	-0.710409	1.634528	-0.752807
C	-2.972019	1.848966	-1.583676
C	-0.511769	3.008670	-0.909500
H	0.083640	1.027299	-0.317488
C	-2.774903	3.222283	-1.742349
H	-3.933817	1.399558	-1.845389
C	-1.545516	3.807715	-1.410630
H	0.448909	3.416701	-0.569997
H	-3.589312	3.841085	-2.129860
H	-1.401238	4.885027	-1.531150
Li	1.827582	1.585091	1.272309
O	2.214476	3.161238	0.789897
H	2.214326	4.108096	0.952553
C	3.325321	-0.903773	0.397197
O	2.536199	0.248292	0.040940
C	3.106811	0.916735	-1.112704
C	4.532194	0.386006	-1.203115
C	4.361939	-1.058665	-0.716414
H	3.806291	-0.717855	1.374629
H	2.662931	-1.777004	0.499609
H	2.518606	0.646459	-2.009440
H	3.023306	1.997670	-0.916535
H	4.947312	0.460242	-2.219332
H	5.190202	0.947572	-0.518849
H	3.961043	-1.687134	-1.528993
H	5.294173	-1.519507	-0.357740
C	0.326151	-0.804255	2.266739
O	0.490715	0.631500	2.255253
C	-0.655125	1.273719	2.852797
C	-1.352197	0.176084	3.648848
C	-1.093702	-1.056305	2.773166
H	0.499937	-1.189750	1.252570

H	1.085289	-1.236965	2.941875
H	-0.301592	2.116837	3.465927
H	-1.305038	1.669504	2.052175
H	-0.874259	0.056338	4.635412
H	-2.420539	0.386213	3.804740
H	-1.176036	-2.008003	3.318186
H	-1.803087	-1.087129	1.932430
27			
D SCF Done: -710.645211674 A.U.			
C	3.346105	-1.772581	0.025120
C	1.972469	-1.695223	0.006950
C	1.361950	-0.416726	-0.035227
C	3.549394	0.645644	-0.059231
C	4.140166	-0.586114	-0.001368
H	3.839013	-2.746257	0.056125
H	1.346948	-2.587631	0.016926
H	4.071032	1.602414	-0.092670
H	5.229283	-0.648235	0.017518
C	0.060699	0.125257	-0.080044
C	-1.250921	-0.536190	-0.069604
C	-1.453738	-1.746854	0.620025
C	-2.340849	0.048537	-0.744176
C	-2.710593	-2.356459	0.627560
H	-0.632609	-2.200291	1.178565
C	-3.597478	-0.558379	-0.725489
H	-2.197892	0.977146	-1.302395
C	-3.786709	-1.765476	-0.043110
H	-2.852172	-3.294073	1.171426
H	-4.431242	-0.089169	-1.253988
H	-4.770111	-2.242433	-0.032448
N	2.177465	0.705108	-0.081177
N	1.459620	1.834682	-0.152785
N	0.198673	1.471295	-0.152411
Li	-1.131525	2.972479	-0.020624
O	-2.031405	4.136773	0.606989
H	-2.549710	4.826698	1.023068
53			
D-THF2 SCF Done: -1175.79183347 A.U.			
C	5.139792	-0.084307	-0.539472
C	4.060470	0.528319	0.055017
C	2.753925	0.128460	-0.323479
C	3.684734	-1.499232	-1.871434
C	4.946004	-1.105611	-1.518898
H	6.155309	0.205327	-0.261714
H	4.185205	1.303021	0.811588
H	3.437991	-2.274277	-2.597505
H	5.801927	-1.588653	-1.992700
C	1.419448	0.439994	0.012381
C	0.902337	1.431330	0.967939
C	1.569825	2.656529	1.161779
C	-0.280821	1.182757	1.690724
C	1.070384	3.606093	2.056577
H	2.469654	2.882962	0.586177
C	-0.777744	2.137415	2.579743
H	-0.819787	0.247038	1.543739
C	-0.106276	3.350655	2.769246

H	1.597639	4.554654	2.188694
H	-1.700509	1.930216	3.128299
H	-0.499507	4.095165	3.466575
N	2.619989	-0.881050	-1.264737
N	1.327807	-1.171669	-1.490573
N	0.624645	-0.377877	-0.721165
Li	-1.443516	-0.859758	-0.806549
O	-2.419853	-1.874567	-1.859627
H	-2.812506	-1.765776	-2.732649
C	-2.625660	-2.751913	0.975221
O	-1.474014	-1.868829	0.956295
C	-0.321768	-2.538063	1.493172
C	-0.869500	-3.751336	2.239368
C	-2.077753	-4.121891	1.370573
H	-3.343966	-2.370121	1.724268
H	-3.057238	-2.716334	-0.039493
H	0.345642	-2.843447	0.666555
H	0.230506	-1.834958	2.137252
H	-0.126333	-4.557383	2.335296
H	-1.197867	-3.461806	3.252016
H	-1.744200	-4.669436	0.473104
H	-2.823275	-4.740443	1.892860
C	-3.658913	0.873909	-1.133549
O	-2.284513	0.985000	-0.709885
C	-1.667552	2.138156	-1.308965
C	-2.784826	2.876275	-2.051342
C	-3.753502	1.736090	-2.386929
H	-3.837885	-0.196391	-1.320240
H	-4.321864	1.251621	-0.331275
H	-1.194585	2.747286	-0.522827
H	-0.875977	1.798924	-2.000938
H	-3.273780	3.604973	-1.383176
H	-2.413835	3.418793	-2.934053
H	-4.779055	2.074187	-2.599243
H	-3.386812	1.163704	-3.255955
27			
B2 SCF Done: -1170.23938728 A.U.			
C	-2.173918	-2.482210	-1.041536
C	-1.348800	-1.369855	-0.889206
C	-1.704569	-0.366484	0.025240
C	-3.634556	-1.528703	0.596987
C	-3.340351	-2.573328	-0.275949
H	-1.908324	-3.272991	-1.747768
H	-0.426880	-1.275025	-1.464532
H	-4.545565	-1.551292	1.204143
H	-4.012858	-3.429621	-0.355790
C	-0.843143	0.881118	0.200931
H	-1.064290	1.293474	1.200609
C	0.643789	0.558734	0.147179
C	1.453371	0.921806	-0.937091
C	1.226825	-0.142148	1.215380
C	2.812232	0.591230	-0.962785
H	1.009328	1.473940	-1.765653
C	2.580336	-0.481146	1.206949
H	0.611425	-0.431626	2.072187
C	3.365275	-0.110337	0.110144
H	3.437823	0.877094	-1.810677

H	3.026476	-1.024209	2.042176
N	-2.845557	-0.450586	0.741948
N	-2.155925	2.658681	-0.643151
N	-1.189925	1.872175	-0.846814
O	-2.847611	2.569323	0.453755
Li	-3.477650	1.286713	1.459618
Cl	5.071036	-0.531083	0.086769
53			
B2-THF2 SCF Done: -1635.40334073 A.U.			
C	0.616544	3.787222	-1.306017
C	1.108015	2.785551	-0.470615
C	0.320649	1.650004	-0.223316
C	-1.374008	2.482799	-1.570436
C	-0.651823	3.635763	-1.875478
H	1.216310	4.677692	-1.512023
H	2.094777	2.872067	-0.013107
H	-2.377570	2.326504	-1.980219
H	-1.075849	4.393787	-2.537269
C	0.783318	0.551134	0.726075
H	0.196624	-0.346976	0.483077
C	2.254676	0.212800	0.547937
C	3.240127	0.646297	1.445328
C	2.649545	-0.552163	-0.562008
C	4.587924	0.333824	1.241335
H	2.939215	1.228641	2.316649
C	3.989790	-0.874349	-0.782047
H	1.895256	-0.905292	-1.269983
C	4.952768	-0.423936	0.126438
H	5.350719	0.675124	1.943923
H	4.286850	-1.472265	-1.645713
N	-0.904135	1.516969	-0.767939
N	-0.626386	0.744198	2.613387
N	0.517284	0.977381	2.123157
O	-1.541525	0.175483	1.895987
Li	-2.071364	0.099259	0.126628
C	-1.428553	-2.728068	0.327648
O	-1.683431	-1.665139	-0.611870
C	-0.947793	-1.888891	-1.833116
C	-0.147526	-3.180572	-1.617915
C	-0.075156	-3.290209	-0.088049
H	-1.448436	-2.290142	1.336287
H	-2.226445	-3.489919	0.246098
H	-1.656311	-1.959821	-2.674913
H	-0.299944	-1.013547	-2.005017
H	-0.691837	-4.043172	-2.034720
H	0.841562	-3.140588	-2.097558
H	0.083511	-4.318894	0.267418
H	0.735636	-2.658954	0.309712
C	-4.693688	0.570407	1.202870
O	-3.974440	0.346909	-0.029985
C	-4.764610	-0.460270	-0.931069
C	-6.106755	-0.681405	-0.227737
C	-5.726256	-0.548346	1.252766
H	-3.959444	0.553644	2.021385
H	-5.177477	1.564389	1.167713
H	-4.861837	0.066652	-1.894631
H	-4.224693	-1.406353	-1.104092

H	-6.823271	0.108675	-0.506535
H	-6.554803	-1.653314	-0.482133
H	-6.579014	-0.309852	1.905515
H	-5.258392	-1.478142	1.617767
Cl	6.644333	-0.821831	-0.138022
27			
TS_B2 SCF Done: -1170.18922036 A.U.			
C	-1.798276	-0.346389	-0.055168
C	-1.438291	-1.715161	-0.198834
C	-2.414661	-2.692865	-0.291495
C	-3.771389	-2.329381	-0.249027
C	-4.060014	-0.980020	-0.111633
N	-3.125031	-0.015106	-0.005859
H	-2.124432	-3.739509	-0.419206
H	-0.387862	-1.993067	-0.268584
H	-4.572093	-3.066587	-0.328584
H	-5.103404	-0.643312	-0.077965
C	-0.790222	0.725486	0.020787
H	-1.414370	1.546164	1.139245
Li	-3.790487	1.683047	0.725766
N	-1.098326	1.904313	-0.795900
N	-1.784640	2.773902	-0.239683
O	-2.131032	2.446975	1.080661
C	0.659109	0.394223	-0.006574
C	1.220443	-0.445079	0.981030
C	1.540871	0.948124	-0.958553
C	2.581609	-0.748062	1.002274
H	0.576410	-0.863800	1.758465
C	2.907494	0.661394	-0.944720
H	1.147302	1.617463	-1.725046
C	3.422768	-0.192075	0.033376
H	2.992744	-1.400814	1.774989
H	3.571071	1.096729	-1.694827
Cl	5.143158	-0.558891	0.057661
53			
TS_B2-THF2 SCF Done: -1635.36334741 A.U.			
C	-0.085146	2.325143	0.291798
C	0.684436	3.496862	0.086827
C	0.184467	4.525431	-0.700595
C	-1.090911	4.399227	-1.273143
C	-1.797739	3.227914	-1.017250
N	-1.317501	2.220235	-0.274133
H	0.774412	5.433133	-0.855894
H	1.655927	3.591795	0.574917
H	-1.525383	5.188649	-1.889453
H	-2.799787	3.082262	-1.437176
C	0.385561	1.220997	1.145116
H	0.469064	1.394164	2.638761
Li	-1.959864	0.287731	-0.085450
N	-0.727084	0.308509	1.487585
N	-0.885168	0.144214	2.727348
O	-0.022128	0.788531	3.490166
C	1.653491	0.516070	0.843307
C	2.544322	0.911679	-0.184434
C	2.013986	-0.648581	1.569834
C	3.713752	0.204828	-0.466569

H	2.316024	1.780343	-0.802337
C	3.177353	-1.365561	1.293618
H	1.371525	-1.007988	2.374397
C	4.030124	-0.937552	0.272580
H	4.371616	0.533428	-1.273990
H	3.421043	-2.260355	1.870343
C	-4.275875	-1.271649	-0.915787
O	-3.666003	-0.533517	0.169247
C	-3.964325	-1.185937	1.418992
C	-4.070050	-2.657868	1.047011
C	-4.798690	-2.583555	-0.303855
H	-5.081722	-0.664559	-1.361424
H	-3.498858	-1.434580	-1.678887
H	-3.160332	-0.947696	2.129710
H	-4.921309	-0.801072	1.819820
H	-3.060157	-3.083496	0.925983
H	-4.609130	-3.251096	1.800277
H	-4.598530	-3.450072	-0.950923
H	-5.886938	-2.525765	-0.143517
C	-0.571421	-2.058352	-1.047020
O	-1.054608	-0.753507	-1.435826
C	-0.226889	-0.199385	-2.481106
C	0.633354	-1.359662	-2.974114
C	0.802937	-2.190850	-1.696459
H	-0.542727	-2.107146	0.052198
H	-1.276912	-2.823094	-1.419513
H	-0.881686	0.230544	-3.255239
H	0.392312	0.607952	-2.056171
H	0.097462	-1.938064	-3.745062
H	1.587934	-1.016564	-3.399600
H	1.077148	-3.238968	-1.886049
H	1.571118	-1.741814	-1.049437
Cl	5.494779	-1.844182	-0.091306

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B3 SCF Done: -789.279212814 A.U.

C	2.127554	-1.940838	1.752928
C	1.231362	-0.986815	1.276282
C	1.531416	-0.284427	0.098660
C	3.543748	-1.429989	-0.107264
C	3.308794	-2.178680	1.043141
H	1.905838	-2.497162	2.667374
H	0.295942	-0.785941	1.800247
H	4.462715	-1.573168	-0.685426
H	4.036457	-2.921956	1.374624
C	0.588871	0.788310	-0.439501
H	0.800160	0.897328	-1.517156
C	-0.872864	0.387222	-0.287116
C	-1.714995	0.973713	0.659498
C	-1.379181	-0.629108	-1.116930
C	-3.053563	0.558314	0.794401
H	-1.320874	1.767748	1.295568
C	-2.703381	-1.064408	-1.006619
H	-0.721636	-1.089828	-1.861052
C	-3.528859	-0.458176	-0.040751
H	-4.567984	-0.789847	0.054505
N	2.685692	-0.503205	-0.566789
N	1.765882	2.823933	-0.176199

N	0.853374	2.069427	0.260858
O	2.478290	2.459736	-1.202120
Li	3.194022	0.976048	-1.783097
C	-3.253136	-2.150492	-1.898190
H	-3.659963	-2.986066	-1.303687
H	-4.081386	-1.771757	-2.521457
H	-2.482838	-2.556433	-2.571248
C	-3.941991	1.213120	1.823420
H	-3.508892	1.128699	2.834518
H	-4.056916	2.291204	1.617893
H	-4.946295	0.763584	1.844693
59			
B3-THF2 SCF Done: -1254.44318956 A.U.			
C	-0.866135	-3.552291	-1.788376
C	-1.328226	-2.642863	-0.839179
C	-0.502267	-1.576196	-0.450294
C	1.173028	-2.299947	-1.881620
C	0.412158	-3.378765	-2.329576
H	-1.495623	-4.388311	-2.104625
H	-2.321764	-2.744464	-0.399425
H	2.184868	-2.132179	-2.265762
H	0.814378	-4.065096	-3.077637
C	-0.940196	-0.587314	0.622300
H	-0.303704	0.302831	0.511644
C	-2.387660	-0.149890	0.448865
C	-3.409421	-0.582241	1.296730
C	-2.703529	0.717179	-0.612831
C	-4.739944	-0.166387	1.099784
H	-3.158240	-1.247353	2.124490
C	-4.014730	1.150509	-0.833611
H	-1.906205	1.057911	-1.279727
C	-5.024743	0.695239	0.034543
H	-6.055607	1.026589	-0.127657
N	0.732206	-1.423326	-0.967353
N	0.410456	-1.100689	2.491726
N	-0.731952	-1.203135	1.956192
O	1.372592	-0.496712	1.869202
Li	1.937472	-0.191195	0.136212
C	1.378086	2.607930	0.716109
O	1.638318	1.676406	-0.352436
C	0.966704	2.097070	-1.558350
C	0.206256	3.380094	-1.197453
C	0.066697	3.279240	0.328335
H	1.335983	2.033025	1.652737
H	2.206226	3.339011	0.775675
H	1.714302	2.252022	-2.353866
H	0.294671	1.282565	-1.874628
H	0.801118	4.267678	-1.466855
H	-0.760473	3.449036	-1.717561
H	-0.070887	4.254378	0.818186
H	-0.784552	2.633771	0.598425
C	4.521988	-0.871710	1.198434
O	3.838401	-0.480449	-0.012369
C	4.669918	0.408558	-0.790833
C	5.996516	0.513463	-0.032701
C	5.573956	0.209224	1.410626
H	3.767285	-0.941234	1.995220

H	4.988160	-1.863795	1.050069
H	4.783600	-0.002552	-1.807555
H	4.154413	1.380847	-0.863105
H	6.705953	-0.251723	-0.388421
H	6.468869	1.499336	-0.155380
H	6.404207	-0.125866	2.049850
H	5.113982	1.097628	1.875215
C	-4.347097	2.103059	-1.955767
H	-5.224177	1.759514	-2.528729
H	-4.595251	3.105037	-1.563638
H	-3.505567	2.218428	-2.655976
C	-5.822696	-0.650050	2.033038
H	-5.875777	-1.752016	2.043178
H	-5.620596	-0.334228	3.070836
H	-6.813453	-0.264588	1.748228
33			
TS_B3 SCF Done: -789.228210192 A.U.			
C	1.613401	0.238760	-0.155246
C	1.331537	1.561968	-0.599761
C	2.360348	2.423017	-0.940337
C	3.694324	1.987441	-0.850515
C	3.905845	0.689099	-0.412745
N	2.919678	-0.161312	-0.064889
H	2.129078	3.430983	-1.296284
H	0.297132	1.887227	-0.698268
H	4.534161	2.631112	-1.117539
H	4.927484	0.298864	-0.325715
C	0.545414	-0.709547	0.194793
H	1.157709	-1.251217	1.476844
Li	3.508193	-1.663504	1.048612
N	0.755124	-2.074890	-0.291576
N	1.409020	-2.815670	0.457613
O	1.822488	-2.180481	1.641144
C	-0.882656	-0.291084	0.090471
C	-1.365688	0.760191	0.901582
C	-1.797136	-0.942794	-0.753504
C	-2.700440	1.172193	0.856180
H	-0.675673	1.258560	1.588578
C	-3.147613	-0.557367	-0.812528
H	-1.450892	-1.769933	-1.377133
C	-3.585254	0.502069	-0.009447
H	-4.635012	0.810635	-0.046137
C	-3.200654	2.305396	1.718981
H	-3.565931	3.143682	1.100748
H	-4.047325	1.984395	2.349344
H	-2.412722	2.694506	2.381680
C	-4.093811	-1.284279	-1.737702
H	-3.751818	-1.223405	-2.785021
H	-4.150197	-2.357066	-1.485414
H	-5.112932	-0.871269	-1.690034
59			
TS_B3-THF2 SCF Done: -1254.40167397 A.U.			
C	-0.427604	2.133531	-0.655322
C	-1.401205	3.164309	-0.626815
C	-1.098540	4.389211	-0.049061
C	0.180601	4.602423	0.490397

C	1.091344	3.553117	0.416023
N	0.805060	2.358973	-0.123267
H	-1.846832	5.186794	-0.032439
H	-2.375423	2.991894	-1.087221
H	0.462459	5.554475	0.944252
H	2.104342	3.669048	0.818962
C	-0.687381	0.832096	-1.288435
H	-0.785135	0.719726	-2.795962
Li	1.783102	0.569965	0.020402
N	0.574686	0.088198	-1.494147
N	0.773408	-0.258843	-2.689056
O	-0.183960	0.078435	-3.535426
C	-1.812044	-0.026260	-0.833171
C	-2.750903	0.375875	0.141390
C	-1.952400	-1.341655	-1.347805
C	-3.782021	-0.468718	0.580850
H	-2.672661	1.363895	0.597649
C	-2.965408	-2.204243	-0.921516
H	-1.252254	-1.702197	-2.102879
C	-3.883688	-1.759136	0.046788
H	-4.679016	-2.429299	0.387857
C	4.343903	-0.364141	1.045975
O	3.614719	0.044396	-0.135081
C	4.028368	-0.762294	-1.255017
C	4.389646	-2.100743	-0.627166
C	5.089786	-1.656105	0.666392
H	5.030171	0.444724	1.348170
H	3.606847	-0.515463	1.849955
H	3.197903	-0.800227	-1.974125
H	4.904565	-0.296610	-1.745082
H	3.469507	-2.664837	-0.401983
H	5.026582	-2.719505	-1.276308
H	5.042119	-2.410855	1.464977
H	6.151735	-1.442013	0.467006
C	0.837901	-1.781319	1.403235
O	1.080466	-0.365379	1.557648
C	0.153928	0.204541	2.507282
C	-0.494791	-0.987699	3.205103
C	-0.500227	-2.039919	2.089192
H	0.830694	-2.019641	0.328753
H	1.661809	-2.336742	1.887155
H	0.712414	0.868659	3.185525
H	-0.592863	0.804536	1.961710
H	0.125089	-1.323781	4.053073
H	-1.499836	-0.749742	3.583717
H	-0.588416	-3.072364	2.458169
H	-1.326424	-1.847323	1.388668
C	-3.072926	-3.606048	-1.472484
H	-2.905043	-4.356991	-0.680824
H	-4.078491	-3.798608	-1.883390
H	-2.338610	-3.790083	-2.271422
C	-4.759290	0.024919	1.621696
H	-5.371738	-0.794034	2.029202
H	-4.238890	0.512606	2.462793
H	-5.448072	0.775704	1.195811

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B4 SCF Done: -825.185484882 A.U.

C	-2.197687	-2.486065	-1.021981
C	-1.356589	-1.388471	-0.853114
C	-1.734501	-0.355412	0.018836
C	-3.715578	-1.464457	0.520251
C	-3.402529	-2.534874	-0.313719
H	-1.915040	-3.298765	-1.696095
H	-0.404339	-1.326674	-1.381404
H	-4.654932	-1.454664	1.083018
H	-4.088938	-3.378666	-0.407531
C	-0.853624	0.876612	0.210115
H	-1.118569	1.316557	1.187100
C	0.626779	0.525206	0.236460
C	1.488775	0.794659	-0.830806
C	1.159530	-0.119863	1.368051
C	2.842955	0.435053	-0.787830
H	1.092618	1.302100	-1.711179
C	2.500023	-0.485092	1.427541
H	0.507892	-0.341360	2.218956
C	3.358908	-0.211210	0.345839
H	3.480401	0.666864	-1.641652
H	2.913429	-0.982731	2.307916
N	-2.911284	-0.399650	0.679705
N	-2.088275	2.659294	-0.741668
N	-1.130016	1.849444	-0.877050
O	-2.836521	2.613222	0.321487
Li	-3.533995	1.366909	1.326788
O	4.648745	-0.601492	0.492571
C	5.568139	-0.350119	-0.554522
H	5.672847	0.730476	-0.760644
H	6.538743	-0.742412	-0.219955
H	5.279496	-0.864706	-1.488991

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B4-THF2 SCF Done: -1290.34908278 A.U.

C	0.610884	3.787801	-1.295006
C	1.110365	2.765164	-0.490797
C	0.316346	1.633489	-0.245318
C	-1.399716	2.510177	-1.537415
C	-0.672193	3.660810	-1.837695
H	1.215508	4.675636	-1.498484
H	2.108977	2.829589	-0.055910
H	-2.414130	2.372242	-1.926712
H	-1.102894	4.435698	-2.475249
C	0.790850	0.512075	0.671006
H	0.180470	-0.371074	0.431636
C	2.251248	0.152737	0.448538
C	3.270586	0.552346	1.318361
C	2.610916	-0.601764	-0.684140
C	4.611535	0.222226	1.078160
H	3.004576	1.126335	2.206850
C	3.936465	-0.938810	-0.938637
H	1.834530	-0.931985	-1.379888
C	4.954396	-0.528151	-0.057162
H	5.374464	0.553363	1.783340
H	4.212642	-1.528195	-1.816157
N	-0.922443	1.524516	-0.763570
N	-0.566004	0.703047	2.599618
N	0.567702	0.922366	2.081472

O	-1.511867	0.160023	1.900439
Li	-2.081277	0.107999	0.143765
C	-1.473783	-2.729931	0.305950
O	-1.745373	-1.658429	-0.619116
C	-1.046148	-1.879990	-1.861869
C	-0.257447	-3.183745	-1.680483
C	-0.140620	-3.305694	-0.154329
H	-1.457430	-2.297735	1.317127
H	-2.282948	-3.481810	0.244725
H	-1.778312	-1.933672	-2.684565
H	-0.391312	-1.011939	-2.043572
H	-0.825695	-4.035791	-2.087063
H	0.717335	-3.152759	-2.189164
H	0.015373	-4.338986	0.188849
H	0.690038	-2.687791	0.222843
C	-4.671834	0.604233	1.283197
O	-3.986457	0.381774	0.031172
C	-4.807694	-0.410351	-0.855165
C	-6.135408	-0.618755	-0.121379
C	-5.717433	-0.501539	1.350313
H	-3.917619	0.571230	2.082880
H	-5.143460	1.604589	1.267935
H	-4.921057	0.123140	-1.813348
H	-4.284048	-1.362101	-1.046034
H	-6.847797	0.182772	-0.377240
H	-6.602500	-1.582760	-0.371648
H	-6.550912	-0.257103	2.025394
H	-5.252963	-1.439995	1.697043
O	6.216238	-0.903513	-0.382716
C	7.286384	-0.528682	0.465093
H	8.201678	-0.936080	0.013095
H	7.386109	0.569204	0.542596
H	7.173888	-0.948235	1.481222

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TS_B4 SCF Done: -825.133919787 A.U.

C	-1.803912	-0.333522	-0.052803
C	-1.418387	-1.705421	-0.058240
C	-2.370182	-2.701804	-0.183849
C	-3.728577	-2.358512	-0.308611
C	-4.042279	-1.008424	-0.290977
N	-3.133338	-0.021507	-0.157917
H	-2.059346	-3.750206	-0.203707
H	-0.363752	-1.967540	0.011262
H	-4.509729	-3.112442	-0.419697
H	-5.087229	-0.687532	-0.383035
C	-0.812380	0.743753	0.060944
H	-1.538342	1.565628	1.119934
Li	-3.874133	1.689789	0.446457
N	-1.058253	1.911970	-0.782160
N	-1.803366	2.778459	-0.298642
O	-2.267865	2.450888	0.987033
C	0.640566	0.393039	0.104385
C	1.183483	-0.253682	1.235513
C	1.528234	0.709756	-0.937186
C	2.531448	-0.591064	1.308043
H	0.527444	-0.496368	2.076240
C	2.890635	0.390775	-0.873884

H	1.147691	1.224125	-1.821929
C	3.404144	-0.270983	0.252121
H	2.940293	-1.094552	2.187477
H	3.536729	0.659897	-1.710370
O	4.703911	-0.629322	0.415032
C	5.632311	-0.329247	-0.609184
H	5.711169	0.758325	-0.790476
H	6.608406	-0.701930	-0.267582
H	5.374774	-0.829744	-1.560607
57			
TS_B4-THF2 SCF Done: -1290.30608925 A.U.			
C	-0.238026	2.211202	0.353417
C	0.518729	3.411561	0.304618
C	0.072893	4.482982	-0.454728
C	-1.136448	4.375321	-1.163121
C	-1.831585	3.174594	-1.064491
N	-1.402995	2.124466	-0.348012
H	0.651867	5.410476	-0.485363
H	1.435039	3.489288	0.892352
H	-1.527221	5.198969	-1.763659
H	-2.780382	3.038133	-1.596788
C	0.168266	1.067972	1.176779
H	0.034182	1.107112	2.697269
Li	-1.979851	0.170576	-0.409501
N	-0.928675	0.081638	1.289971
N	-1.238043	-0.206957	2.476543
O	-0.519577	0.405639	3.405737
C	1.506709	0.437251	0.991399
C	2.467676	0.898459	0.067555
C	1.858902	-0.730624	1.717085
C	3.701531	0.262178	-0.120641
H	2.253717	1.771512	-0.550307
C	3.075390	-1.378905	1.529368
H	1.163587	-1.144609	2.448627
C	4.019432	-0.891643	0.609610
H	4.395560	0.672374	-0.855429
H	3.319301	-2.280259	2.097416
C	-4.377722	-0.684597	0.951240
O	-3.756531	-0.547442	-0.337273
C	-4.060943	-1.759019	-1.044224
C	-3.926487	-2.876973	0.003043
C	-4.121623	-2.142600	1.357574
H	-3.928250	0.054097	1.629173
H	-5.458545	-0.471934	0.852883
H	-5.093107	-1.696811	-1.436146
H	-3.364606	-1.838710	-1.890403
H	-4.670410	-3.669799	-0.163248
H	-2.928547	-3.336164	-0.049794
H	-4.956982	-2.547992	1.946897
H	-3.211015	-2.201655	1.970880
C	-0.411094	-2.097941	-1.312622
O	-0.940007	-0.810298	-1.703722
C	-0.028746	-0.146727	-2.608207
C	0.977394	-1.214884	-3.028080
C	1.042249	-2.097829	-1.775801
H	-0.523288	-2.204585	-0.223137
H	-0.998782	-2.888760	-1.812440

H	-0.609214	0.272216	-3.445145
H	0.464993	0.681483	-2.073060
H	0.595409	-1.789032	-3.888600
H	1.949702	-0.781147	-3.304852
H	1.417612	-3.112859	-1.972283
H	1.682850	-1.631378	-1.012751
O	5.182030	-1.591760	0.498644
C	6.155436	-1.151335	-0.425031
H	6.518939	-0.133243	-0.191942
H	7.000040	-1.851537	-0.352712
H	5.776183	-1.160723	-1.463988
35			
B5 SCF Done: -844.637333339 A.U.			
C	2.431696	2.462094	-1.163554
C	1.648452	1.328690	-0.958862
C	2.035364	0.385382	0.006339
C	3.914771	1.651431	0.530464
C	3.588024	2.637907	-0.396258
H	2.141501	3.205151	-1.910878
H	0.732762	1.169402	-1.529677
H	4.818596	1.740493	1.142437
H	4.226997	3.515115	-0.515330
C	1.216068	-0.881053	0.244599
H	1.460858	-1.237046	1.260612
C	-0.280358	-0.619638	0.179814
C	-1.067438	-0.953342	-0.930515
C	-0.922569	0.016145	1.253360
C	-2.431923	-0.664295	-0.976959
H	-0.596190	-1.457640	-1.775549
C	-2.283061	0.315696	1.229203
H	-0.341418	0.290889	2.139869
C	-3.085446	-0.017535	0.104591
H	-2.990616	-0.950955	-1.867548
H	-2.722710	0.807845	2.096188
N	3.167253	0.551199	0.724015
N	2.597434	-2.644245	-0.529115
N	1.600215	-1.906657	-0.759772
O	3.293513	-2.481064	0.558693
Li	3.844848	-1.132081	1.518443
N	-4.433775	0.271570	0.068759
C	-5.059859	0.955275	1.182440
H	-4.619678	1.954613	1.361883
H	-6.128211	1.093615	0.973249
H	-4.974812	0.381640	2.124101
C	-5.217632	-0.066564	-1.102330
H	-4.853798	0.446664	-2.012644
H	-5.209017	-1.152907	-1.308806
H	-6.261334	0.233651	-0.943977
61			
B5-THF2 SCF Done: -1309.80075225 A.U.			
C	0.240937	3.793450	-1.429615
C	0.753585	2.836426	-0.556313
C	0.002105	1.682203	-0.281689
C	-1.699436	2.413401	-1.680367
C	-1.012759	3.579875	-2.013010
H	0.812845	4.697408	-1.655710

H	1.731114	2.967749	-0.089833
H	-2.690398	2.208698	-2.099710
H	-1.451605	4.300856	-2.705874
C	0.494442	0.628182	0.703128
H	-0.073868	-0.289656	0.491950
C	1.973732	0.320923	0.542621
C	2.960610	0.845139	1.388401
C	2.403791	-0.508197	-0.505188
C	4.314818	0.565473	1.199684
H	2.653399	1.479231	2.221739
C	3.750607	-0.800998	-0.713763
H	1.663102	-0.943106	-1.182879
C	4.755124	-0.263620	0.134924
H	5.033871	0.998946	1.894391
H	4.017485	-1.457455	-1.541519
N	-1.209991	1.491309	-0.838424
N	-0.929504	0.865714	2.579279
N	0.211409	1.099050	2.084668
O	-1.834629	0.255014	1.880629
Li	-2.344069	0.085601	0.113432
C	-1.656882	-2.711692	0.458187
O	-1.928111	-1.706837	-0.539170
C	-1.166224	-1.969336	-1.736272
C	-0.348920	-3.235878	-1.451137
C	-0.288680	-3.266566	0.082772
H	-1.693181	-2.220263	1.441418
H	-2.438135	-3.493600	0.412742
H	-1.858342	-2.087875	-2.586318
H	-0.528471	-1.091992	-1.933878
H	-0.876618	-4.126678	-1.828471
H	0.643806	-3.203900	-1.923851
H	-0.113302	-4.272540	0.491548
H	0.505898	-2.599479	0.453776
C	-4.980201	0.547607	1.162531
O	-4.255515	0.282348	-0.058415
C	-5.025020	-0.587365	-0.917845
C	-6.358722	-0.813880	-0.199778
C	-5.979891	-0.596567	1.271153
H	-4.244880	0.593320	1.978943
H	-5.493164	1.523958	1.077811
H	-5.140587	-0.108739	-1.904388
H	-4.458601	-1.524464	-1.049500
H	-7.099382	-0.060524	-0.514796
H	-6.777709	-1.810208	-0.404514
H	-6.838189	-0.350872	1.913942
H	-5.484495	-1.493146	1.680340
C	6.499032	-1.446147	-1.117751
H	7.593858	-1.523144	-1.132972
H	6.089621	-2.465800	-0.979964
H	6.176772	-1.091779	-2.113764
C	7.081034	-0.040147	0.872300
H	6.920988	-0.422360	1.898973
H	8.081931	-0.353858	0.549323
H	7.078813	1.063760	0.926080
N	6.093396	-0.538531	-0.063741

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TS_B5 SCF Done: -844.585557654 A.U.

C	2.113330	0.354987	-0.055557
C	1.652242	1.703433	-0.105792
C	2.550120	2.747071	-0.238857
C	3.928868	2.477037	-0.323965
C	4.316598	1.147929	-0.259430
N	3.460615	0.115267	-0.120595
H	2.183038	3.775969	-0.293168
H	0.582831	1.904841	-0.060959
H	4.669230	3.270618	-0.438407
H	5.379977	0.883427	-0.315029
C	1.177064	-0.766193	0.073128
H	1.910486	-1.484478	1.199021
Li	4.268985	-1.525658	0.569694
N	1.512563	-1.963719	-0.691935
N	2.288833	-2.759275	-0.138875
O	2.695876	-2.332198	1.137985
C	-0.293018	-0.486034	0.033452
C	-0.947926	0.078709	1.142168
C	-1.094585	-0.781408	-1.084096
C	-2.313098	0.364017	1.137373
H	-0.367794	0.304362	2.042225
C	-2.464278	-0.519549	-1.105100
H	-0.633429	-1.238795	-1.962737
C	-3.118292	0.077513	0.004141
H	-2.753578	0.802861	2.032353
H	-3.026005	-0.780424	-2.001916
C	-5.123194	0.845987	1.184558
H	-6.185977	1.025754	0.976997
H	-5.057764	0.128832	2.026658
H	-4.687442	1.800945	1.528817
C	-5.280979	-0.061758	-1.140738
H	-4.928890	0.384842	-2.087593
H	-5.286593	-1.161670	-1.274674
H	-6.317952	0.265019	-0.989179
N	-4.472185	0.359444	-0.014747
61			
TS_B5-THF2 SCF Done: -1309.75743388 A.U.			
C	-0.806256	1.931108	0.586833
C	-0.310921	3.239637	0.838445
C	-0.938999	4.339881	0.276441
C	-2.073642	4.153902	-0.534400
C	-2.506497	2.848115	-0.737353
N	-1.898088	1.772362	-0.215217
H	-0.562657	5.346946	0.478374
H	0.547402	3.366884	1.500499
H	-2.602750	4.995033	-0.986369
H	-3.384061	2.646091	-1.363248
C	-0.211926	0.743534	1.199272
H	-0.459220	0.420512	2.675856
Li	-2.041962	-0.192364	-0.744061
N	-1.067520	-0.446517	0.989452
N	-1.386747	-1.042719	2.051230
O	-0.892205	-0.511590	3.162068
C	1.243168	0.449116	1.035202
C	2.126845	1.251941	0.282198
C	1.809982	-0.730878	1.569606
C	3.468520	0.920826	0.086666

H	1.759856	2.160202	-0.198852
C	3.144116	-1.083960	1.369922
H	1.188921	-1.409090	2.157626
C	4.029614	-0.258941	0.633375
H	4.076252	1.594026	-0.518112
H	3.495069	-2.019668	1.804953
C	-3.806251	-2.451078	-0.662045
O	-3.767974	-1.009114	-0.711190
C	-4.681530	-0.455085	0.268550
C	-5.407807	-1.652312	0.884833
C	-4.383111	-2.780384	0.708770
H	-4.451890	-2.826349	-1.477550
H	-2.786043	-2.833575	-0.821378
H	-4.091449	0.096772	1.018931
H	-5.356257	0.254471	-0.236549
H	-5.684563	-1.472398	1.933956
H	-6.327394	-1.879543	0.320712
H	-3.592614	-2.702753	1.472147
H	-4.824130	-3.787144	0.752281
C	-0.037361	-1.897759	-1.937497
O	-0.783436	-0.673009	-2.114185
C	0.039397	0.328778	-2.754329
C	1.285982	-0.410918	-3.234852
C	1.419738	-1.523382	-2.187825
H	-0.221352	-2.273350	-0.919330
H	-0.401275	-2.644207	-2.666831
H	-0.541272	0.794298	-3.566430
H	0.293450	1.105562	-2.014181
H	1.119652	-0.839504	-4.237176
H	2.165136	0.248609	-3.281320
H	2.018881	-2.379808	-2.530444
H	1.871429	-1.127158	-1.266029
C	5.818233	-1.920316	0.816616
H	5.661914	-2.122168	1.889833
H	5.302049	-2.722362	0.249022
H	6.895709	-2.007047	0.622550
C	6.159817	0.158876	-0.499022
H	5.775798	0.083180	-1.537886
H	6.197711	1.230034	-0.238071
H	7.192936	-0.213952	-0.490730
N	5.368482	-0.591688	0.453957

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B6 SCF Done: -789.277552136 A.U.

C	2.282733	-2.209198	0.900955
C	1.345273	-1.168792	0.925767
C	1.404744	-0.221761	-0.124896
C	3.255730	-1.279063	-1.072235
C	3.240255	-2.285183	-0.112105
H	2.262011	-2.964947	1.691430
H	4.010629	-1.267012	-1.865231
H	3.972791	-3.094266	-0.143687
C	0.413631	0.936706	-0.235455
H	0.582089	1.396722	-1.226614
C	-1.044049	0.488525	-0.218631
C	-2.023197	1.174419	0.508243
C	-1.445331	-0.612054	-0.994910
C	-3.361068	0.763978	0.472111

H	-1.727265	2.031788	1.114399
C	-2.778706	-1.020303	-1.027118
H	-0.702582	-1.162525	-1.579728
C	-3.765791	-0.340943	-0.290110
H	-4.105302	1.316640	1.053590
H	-3.062868	-1.883999	-1.636474
N	2.366256	-0.274192	-1.070884
N	1.603886	2.775969	0.633804
N	0.671268	1.942387	0.818358
O	2.317556	2.717934	-0.449640
Li	2.796322	1.569242	-1.683003
C	-5.202733	-0.797781	-0.329321
H	-5.853584	-0.148433	0.275524
H	-5.592452	-0.802275	-1.361573
H	-5.303967	-1.828075	0.053036
C	0.330655	-1.086737	2.036253
H	0.171737	-0.047343	2.353597
H	-0.645994	-1.482337	1.712907
H	0.662604	-1.675173	2.904718

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B6-THF2 SCF Done: -1254.44156568 A.U.

C	0.779254	3.946094	-0.892279
C	1.259916	2.897367	-0.097983
C	0.517327	1.692203	-0.103203
C	-1.072929	2.584775	-1.548445
C	-0.392315	3.795978	-1.637415
H	1.327712	4.892222	-0.918656
H	-2.013761	2.424069	-2.085305
H	-0.778242	4.606313	-2.259574
C	0.927990	0.475954	0.718671
H	0.251926	-0.335494	0.414346
C	2.333350	-0.034398	0.436257
C	3.126697	-0.589761	1.447416
C	2.830895	-0.056041	-0.878229
C	4.379844	-1.141505	1.156039
H	2.755007	-0.582643	2.473406
C	4.080831	-0.605760	-1.165926
H	2.233817	0.367407	-1.690589
C	4.883471	-1.159947	-0.152462
H	4.978187	-1.567029	1.967482
H	4.443672	-0.606006	-2.198596
N	-0.628719	1.566282	-0.800385
N	-0.438074	0.582560	2.630605
N	0.729482	0.742935	2.162541
O	-1.406902	0.221983	1.852033
Li	-1.854184	0.140402	0.045084
C	-1.320317	-2.695809	0.305448
O	-1.451959	-1.646159	-0.674437
C	-0.563599	-1.888809	-1.788065
C	0.193902	-3.180996	-1.456383
C	0.072696	-3.267249	0.072000
H	-1.462960	-2.242944	1.297589
H	-2.105568	-3.456421	0.136186
H	-1.158236	-1.964137	-2.713299
H	0.111050	-1.022360	-1.881002
H	-0.298433	-4.047714	-1.926370
H	1.236115	-3.148236	-1.806014

H	0.179904	-4.290991	0.459751
H	0.830734	-2.632596	0.558872
C	-4.517390	0.377984	1.103243
O	-3.764307	0.326419	-0.127554
C	-4.492065	-0.427657	-1.123233
C	-5.794734	-0.873234	-0.447962
C	-5.425144	-0.842890	1.041283
H	-3.794294	0.374549	1.931297
H	-5.105043	1.314885	1.135187
H	-4.662160	0.209386	-2.007126
H	-3.864128	-1.282797	-1.422607
H	-6.601931	-0.150574	-0.651016
H	-6.127335	-1.861457	-0.798531
H	-6.296486	-0.760352	1.707766
H	-4.858018	-1.747127	1.319905
C	2.514440	3.065480	0.719112
H	2.410770	2.587422	1.702745
H	3.379197	2.598225	0.219573
H	2.744190	4.131796	0.864658
C	6.237458	-1.740872	-0.475830
H	6.169179	-2.494641	-1.278346
H	6.931360	-0.959470	-0.831596
H	6.695379	-2.220330	0.402641

33

TS_B6 SCF Done: -789.219155284 A.U.

C	1.509875	-0.186115	0.048404
C	1.399109	-1.578105	0.396928
C	2.517021	-2.393237	0.212882
C	3.740372	-1.873551	-0.225829
C	3.800911	-0.503989	-0.433170
N	2.738000	0.307354	-0.315456
H	2.443525	-3.453939	0.471813
H	4.623100	-2.502556	-0.353443
H	4.749849	-0.029737	-0.713248
C	0.386069	0.767004	0.119822
H	0.830372	1.834804	-0.965501
Li	3.112943	2.127599	-0.941581
N	0.621063	1.898163	1.034674
N	1.135021	2.906739	0.542380
O	1.379701	2.790359	-0.851846
C	-1.030770	0.366900	0.046264
C	-1.473436	-0.506539	-0.975612
C	-2.025589	0.901984	0.894445
C	-2.816267	-0.853673	-1.109915
H	-0.741572	-0.914846	-1.678509
C	-3.370671	0.552929	0.748915
H	-1.735598	1.596823	1.685508
C	-3.800936	-0.334848	-0.249607
H	-3.112001	-1.538068	-1.912000
H	-4.107115	0.983423	1.435404
C	0.182743	-2.181750	1.052254
H	-0.281356	-1.482454	1.761965
H	-0.601070	-2.454515	0.328167
H	0.465011	-3.093708	1.600048
C	-5.256326	-0.690720	-0.427194
H	-5.850774	-0.424548	0.460855
H	-5.699740	-0.160638	-1.289680

H	-5.390287	-1.769237	-0.614570
59			
TS_B6-THF2 SCF Done: -1254.40066235 A.U.			
C	0.619631	2.062034	0.051266
C	1.608291	3.074530	-0.143933
C	1.331217	4.084771	-1.067491
C	0.112347	4.115961	-1.756010
C	-0.812295	3.115364	-1.473553
N	-0.567420	2.122312	-0.610375
H	2.069980	4.875412	-1.231310
H	-0.119027	4.905829	-2.473477
H	-1.791858	3.103046	-1.965481
C	0.813256	0.958352	1.011334
H	0.971700	1.194732	2.527823
Li	-1.691059	0.476605	-0.166699
N	-0.488582	0.394458	1.427312
N	-0.656136	0.345023	2.673840
O	0.367276	0.785795	3.393902
C	1.838565	-0.080479	0.744282
C	2.688021	-0.050290	-0.386367
C	1.982310	-1.205254	1.597278
C	3.629562	-1.054293	-0.630736
H	2.594728	0.761893	-1.109942
C	2.915622	-2.207773	1.339115
H	1.351460	-1.295166	2.483003
C	3.770324	-2.157898	0.223298
H	4.258567	-0.982761	-1.524098
H	2.982736	-3.057541	2.026616
C	-4.396070	-0.393219	-0.817367
O	-3.564632	0.258578	0.171808
C	-4.011987	-0.106069	1.492592
C	-4.595560	-1.499857	1.311325
C	-5.306716	-1.360770	-0.042965
H	-4.965749	0.369940	-1.373562
H	-3.725503	-0.910903	-1.521236
H	-3.150298	-0.053615	2.173012
H	-4.781433	0.611617	1.835294
H	-3.779772	-2.239448	1.252195
H	-5.269751	-1.790614	2.130407
H	-5.433341	-2.319189	-0.567446
H	-6.305562	-0.918270	0.099132
C	-1.039457	-2.278789	-0.755968
O	-1.192288	-0.967411	-1.340727
C	-0.316474	-0.815685	-2.479063
C	0.214117	-2.216747	-2.773794
C	0.231327	-2.849783	-1.376936
H	-0.981472	-2.168166	0.337573
H	-1.927956	-2.886621	-1.007164
H	-0.892479	-0.375538	-3.308451
H	0.498142	-0.123664	-2.210008
H	-0.478283	-2.760971	-3.437517
H	1.204472	-2.192121	-3.251886
H	0.232394	-3.949659	-1.392221
H	1.112513	-2.507550	-0.814168
C	2.877199	3.095641	0.662398
H	3.576003	2.296983	0.364667
H	3.399401	4.058521	0.556630

H	2.657184	2.925637	1.729664
C	4.791279	-3.239608	-0.027869
H	5.638437	-3.168223	0.678074
H	4.356297	-4.245143	0.099567
H	5.206701	-3.177331	-1.045918
42			
B6_tBu SCF Done: -906.264491167 A.U.			
C	2.374518	-1.774721	-0.897639
C	1.471525	-1.059230	-0.084357
C	1.320999	0.323830	-0.415375
C	3.007201	0.193579	-2.059835
C	3.134622	-1.178091	-1.898060
H	2.494263	-2.845831	-0.747220
H	3.617888	0.746212	-2.782028
H	3.822877	-1.760563	-2.513589
C	0.263011	1.328903	0.094481
H	0.367545	2.182190	-0.597756
C	-1.172095	0.853175	-0.105713
C	-2.156887	0.983927	0.878952
C	-1.550301	0.329674	-1.354858
C	-3.470225	0.562080	0.637653
H	-1.888310	1.417461	1.843151
C	-2.859169	-0.084983	-1.593649
H	-0.804433	0.233020	-2.149068
C	-3.846671	0.013492	-0.595999
H	-4.217983	0.665630	1.429753
H	-3.124067	-0.496734	-2.572480
N	2.125811	0.899440	-1.347217
N	1.321423	2.760466	1.644248
N	0.477803	1.837982	1.463805
O	2.013968	3.215619	0.644077
Li	2.441260	2.824540	-0.999136
C	-5.254549	-0.457637	-0.861392
H	-5.921123	-0.250029	-0.010723
H	-5.678884	0.032362	-1.754074
H	-5.280260	-1.544358	-1.052490
C	0.759133	-1.873726	1.037206
C	0.515374	-1.054577	2.316149
H	1.456312	-0.635531	2.706470
H	-0.172244	-0.220161	2.170341
H	0.088019	-1.712502	3.090090
C	-0.579642	-2.444998	0.516095
H	-1.320357	-1.660572	0.325430
H	-0.430394	-3.011072	-0.417758
H	-1.004047	-3.134190	1.264902
C	1.634071	-3.078996	1.468140
H	1.700552	-3.865355	0.701722
H	2.656418	-2.767799	1.737118
H	1.181939	-3.546178	2.356354
68			
B6_tBu-THF2 SCF Done: -1372.41945099 A.U.			
C	-0.768622	-3.325352	-1.517768
C	-1.167266	-2.478857	-0.464037
C	-0.467740	-1.237835	-0.385609
C	0.944142	-1.810423	-2.172124
C	0.266456	-3.002127	-2.392095

H	-1.270797	-4.279981	-1.662470
H	1.809071	-1.519383	-2.777748
H	0.552400	-3.674461	-3.203712
C	-0.761890	-0.044416	0.532294
H	0.034939	0.670655	0.285355
C	-2.033036	0.722730	0.192960
C	-3.738629	2.344231	0.821670
C	-3.641375	1.549282	-1.441633
C	-4.262904	2.363039	-0.482328
H	-4.197277	2.971421	1.592714
H	-4.020038	1.542847	-2.468282
N	0.577024	-0.969112	-1.204102
N	0.517747	-0.428402	2.455068
N	-0.653589	-0.324839	1.976692
O	1.544423	-0.326538	1.676469
Li	2.004466	0.052232	-0.090306
C	2.089556	2.800508	0.783463
O	1.948522	1.985908	-0.389112
C	1.092134	2.687366	-1.305861
C	0.160711	3.568919	-0.443368
C	0.698762	3.395511	0.996066
H	2.427861	2.150498	1.602555
H	2.848255	3.585431	0.599369
H	1.714598	3.298094	-1.984194
H	0.560424	1.932025	-1.902823
H	0.212785	4.617814	-0.770934
H	-0.886544	3.244697	-0.518942
H	0.731646	4.339226	1.559876
H	0.075557	2.685655	1.560462
C	4.561524	-0.940612	0.798480
O	3.836215	-0.460978	-0.354705
C	4.710455	0.312552	-1.207302
C	6.090100	0.273647	-0.541414
C	5.740095	0.014640	0.930079
H	3.866683	-0.936930	1.650351
H	4.902076	-1.976322	0.611308
H	4.707202	-0.124866	-2.219444
H	4.305629	1.336433	-1.267819
H	6.687798	-0.562341	-0.940144
H	6.655329	1.203462	-0.702556
H	6.571289	-0.413314	1.509853
H	5.416462	0.947171	1.422429
C	-2.202348	-3.034316	0.553242
C	-5.460250	3.215557	-0.821481
H	-5.613144	3.289752	-1.909121
H	-6.383286	2.795512	-0.384190
H	-5.353957	4.236991	-0.420289
C	-2.644579	1.543229	1.153577
H	-2.256189	1.540357	2.173652
C	-2.545419	0.744776	-1.111612
H	-2.087570	0.127894	-1.888576
C	-3.210873	-1.995542	1.077581
H	-3.945811	-2.505725	1.721141
H	-2.726061	-1.227311	1.687402
H	-3.760294	-1.510897	0.257269
C	-3.034199	-4.185000	-0.057901
H	-3.796891	-4.501878	0.669829
H	-3.557657	-3.868425	-0.974948

H	-2.433954	-5.077031	-0.291276
C	-1.400070	-3.607542	1.747027
H	-0.695323	-4.385864	1.411480
H	-0.830883	-2.818983	2.257733
H	-2.087683	-4.063388	2.479366
42			
TS_B6_tBu SCF Done: -906.226134268 A.U.			
C	-1.129209	0.374941	0.698135
C	-2.013453	-0.599930	0.141477
C	-2.924144	-1.187590	1.035840
C	-3.023428	-0.781597	2.367999
C	-2.208285	0.260218	2.787796
N	-1.287433	0.800554	1.982174
H	-3.600453	-1.968693	0.692210
H	-3.740638	-1.243847	3.049207
H	-2.281914	0.668422	3.801744
C	0.026436	1.000540	-0.019123
H	0.185350	1.601204	-1.498783
Li	-0.260685	2.478029	2.230991
N	0.100966	2.425737	0.330567
N	0.332848	3.211243	-0.627485
O	0.492099	2.602739	-1.804046
C	1.324674	0.292877	0.076626
C	1.414941	-1.066314	0.471040
C	2.556124	0.936540	-0.208042
C	2.636581	-1.735132	0.537864
H	0.507169	-1.611426	0.735249
C	3.774463	0.257783	-0.130796
H	2.567381	1.987725	-0.499928
C	3.850483	-1.095456	0.233669
H	2.647074	-2.785910	0.846813
H	4.695645	0.802659	-0.362924
C	-2.107972	-0.924043	-1.373394
C	5.163319	-1.837979	0.276241
H	5.327512	-2.424643	-0.646293
H	6.016987	-1.149043	0.377710
H	5.200691	-2.550386	1.117066
C	-2.533663	0.365980	-2.114352
H	-3.502968	0.732748	-1.739047
H	-1.794967	1.168966	-1.994496
H	-2.641734	0.164123	-3.192983
C	-0.788653	-1.456356	-1.968862
H	0.018598	-0.718643	-1.913268
H	-0.455638	-2.368817	-1.450648
H	-0.941634	-1.710315	-3.030683
C	-3.185929	-1.990344	-1.660003
H	-2.957190	-2.952346	-1.173723
H	-4.191059	-1.671548	-1.342591
H	-3.231326	-2.173794	-2.744700
68			
TS_B6_tBu-THF2 SCF Done: -1372.37918760 A.U.			
C	-1.016925	-1.408790	-0.186376
C	-2.305538	-1.930993	-0.535552
C	-2.353415	-2.726704	-1.694368
C	-1.211832	-3.089051	-2.407910
C	0.008948	-2.638571	-1.918282

N	0.091981	-1.818461	-0.871665
H	-3.315929	-3.106438	-2.042096
H	-1.269397	-3.720705	-3.296628
H	0.953457	-2.925693	-2.395701
C	-0.749271	-0.414545	0.881791
H	-1.083609	-0.589383	2.393290
Li	1.783591	-0.922033	-0.189452
N	0.633882	-0.543292	1.382975
N	0.732982	-0.609021	2.634446
O	-0.426412	-0.539186	3.288842
C	-1.158554	0.989689	0.666978
C	-1.923068	1.400368	-0.452669
C	-0.782095	2.022005	1.566262
C	-2.306648	2.729673	-0.641386
H	-2.210117	0.664330	-1.204648
C	-1.165682	3.348300	1.365808
H	-0.180681	1.783142	2.444461
C	-1.944088	3.740383	0.263348
H	-2.893995	2.988544	-1.528775
H	-0.845930	4.104430	2.090618
C	4.626735	-1.284240	-0.718632
O	3.541454	-1.588598	0.188815
C	4.026178	-1.560332	1.545863
C	5.160068	-0.545777	1.510124
C	5.818386	-0.868580	0.160408
H	4.845764	-2.172135	-1.335178
H	4.283913	-0.473845	-1.381119
H	3.188097	-1.289585	2.203530
H	4.392842	-2.564969	1.830291
H	4.744588	0.475683	1.509850
H	5.846561	-0.641590	2.364238
H	6.371443	-0.019358	-0.266979
H	6.522879	-1.707730	0.275264
C	2.440553	1.893871	-0.509421
O	2.037040	0.694316	-1.204535
C	1.281520	1.026073	-2.389475
C	1.501313	2.521017	-2.601592
C	1.646214	3.022727	-1.159713
H	2.224141	1.767887	0.562560
H	3.529794	2.029766	-0.639513
H	1.641868	0.399592	-3.220622
H	0.218104	0.797502	-2.209872
H	2.429445	2.699017	-3.170151
H	0.666955	2.989916	-3.143747
H	2.156181	3.994019	-1.079439
H	0.657008	3.107812	-0.685608
C	-3.653775	-1.786958	0.233241
C	-3.588843	-1.101033	1.609847
H	-2.912733	-1.628800	2.296770
H	-3.280355	-0.051437	1.549515
H	-4.596704	-1.123643	2.056382
C	-4.668522	-1.009587	-0.636942
H	-5.652689	-0.985862	-0.140066
H	-4.346907	0.031200	-0.789700
H	-4.807429	-1.473605	-1.625891
C	-4.209443	-3.212268	0.495843
H	-5.150446	-3.149550	1.066108
H	-4.427612	-3.765862	-0.429110

H	-3.495020	-3.808755	1.086403
C	-2.383165	5.171307	0.075095
H	-3.316157	5.386150	0.628086
H	-1.623794	5.881032	0.441988
H	-2.577177	5.400272	-0.985160
39			
B6_mes SCF Done: -866.989146390 A.U.			
C	2.425452	-1.923158	1.521385
C	1.437767	-0.962801	1.266851
C	1.533484	-0.242431	0.052318
C	3.516390	-1.334108	-0.517336
C	3.470606	-2.132352	0.620440
H	2.374945	-2.508336	2.444015
H	4.335386	-1.426864	-1.238423
H	4.243373	-2.880863	0.806263
C	0.513780	0.822332	-0.366913
H	0.695112	1.009216	-1.438530
C	-0.954001	0.381287	-0.266490
C	-1.967835	1.050022	0.468284
C	-1.316008	-0.764880	-1.030631
C	-3.272224	0.519342	0.465222
C	-2.629386	-1.248844	-0.998906
C	-3.629544	-0.629041	-0.242900
H	-4.041171	1.039542	1.044175
H	-2.879099	-2.134549	-1.591780
N	2.576744	-0.415802	-0.787221
N	1.698579	2.845607	-0.100436
N	0.852688	2.045469	0.392874
O	2.261451	2.584731	-1.246806
Li	2.909670	1.133972	-1.984266
C	-5.033749	-1.178591	-0.217957
H	-5.707331	-0.551031	0.385145
H	-5.453870	-1.247180	-1.235885
H	-5.054676	-2.198509	0.203212
C	0.340057	-0.726311	2.269813
H	0.153496	0.347715	2.402052
H	-0.607870	-1.185814	1.948424
H	0.611441	-1.155834	3.245641
C	-1.777219	2.319635	1.272984
H	-1.082626	2.183574	2.113792
H	-1.357624	3.134124	0.667231
H	-2.745833	2.651457	1.677988
C	-0.326174	-1.507871	-1.902280
H	0.308775	-0.829056	-2.492068
H	0.356151	-2.137828	-1.308946
H	-0.853646	-2.169825	-2.604892
65			
B6_mes-THF2 SCF Done: -1333.09827184 A.U.			
C	-0.330128	-3.494912	-1.745630
C	-0.973852	-2.690817	-0.796157
C	-0.314089	-1.500404	-0.406712
C	1.511031	-1.973489	-1.773077
C	0.921216	-3.139111	-2.254042
H	-0.814290	-4.417102	-2.080321
H	2.508531	-1.660002	-2.098160
H	1.433718	-3.760826	-2.991286

C	-0.874831	-0.538561	0.642893
H	-0.268470	0.376764	0.560878
C	-2.329177	-0.099643	0.420154
C	-3.372095	-0.192300	1.378923
C	-2.618989	0.509421	-0.834715
C	-4.659569	0.261177	1.032143
C	-3.916787	0.946784	-1.126292
C	-4.965291	0.820336	-0.209538
H	-5.454873	0.173824	1.778529
H	-4.111329	1.406977	-2.100506
N	0.904018	-1.181394	-0.881280
N	0.510538	-0.967824	2.506931
N	-0.606633	-1.185413	1.947256
O	1.390698	-0.196861	1.946625
Li	1.954684	0.178744	0.233077
C	1.119199	2.915268	0.882428
O	1.698047	2.063822	-0.116895
C	1.630376	2.747128	-1.378418
C	0.467293	3.760991	-1.260024
C	-0.071454	3.546841	0.170671
H	0.867086	2.284464	1.745760
H	1.858420	3.678393	1.195112
H	2.592309	3.254388	-1.571620
H	1.477742	1.988563	-2.161106
H	0.841601	4.787569	-1.390551
H	-0.307005	3.588390	-2.020987
H	-0.404956	4.479113	0.649424
H	-0.916656	2.841004	0.169352
C	4.417983	-1.180861	0.732987
O	3.814995	-0.180508	-0.118404
C	4.765242	0.860287	-0.426767
C	6.115625	0.333800	0.055571
C	5.704743	-0.542086	1.245987
H	3.697613	-1.431538	1.526137
H	4.623030	-2.085799	0.132736
H	4.730535	1.061248	-1.509452
H	4.470717	1.780853	0.106771
H	6.590151	-0.282283	-0.726286
H	6.809447	1.144506	0.322734
H	6.462488	-1.288159	1.527148
H	5.491664	0.084918	2.127703
C	-2.305207	-3.103362	-0.225562
H	-2.325497	-2.960318	0.863478
H	-3.128755	-2.505447	-0.647448
H	-2.509173	-4.162590	-0.442770
C	-6.355868	1.292366	-0.553476
H	-6.364437	2.369967	-0.791462
H	-6.746635	0.768168	-1.442430
H	-7.060908	1.124052	0.274750
C	-1.566160	0.712097	-1.903220
H	-1.894229	1.472500	-2.627354
H	-0.602698	1.031310	-1.487983
H	-1.371451	-0.214615	-2.467321
C	-3.225486	-0.742361	2.783548
H	-2.413942	-0.252814	3.338039
H	-4.165085	-0.597057	3.339344
H	-2.986442	-1.815423	2.788912

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TS_B6_mes SCF Done: -866.946528409 A.U.

C	1.618381	-0.127825	0.025222
C	1.742738	-1.078427	1.095256
C	2.922327	-1.807206	1.185344
C	3.970106	-1.617883	0.265556
C	3.778722	-0.677074	-0.734384
N	2.644932	0.031838	-0.867921
H	3.042249	-2.524075	2.003797
H	4.903041	-2.180054	0.336360
H	4.561068	-0.485229	-1.477918
C	0.458802	0.739133	-0.115641
H	0.936849	1.923076	0.865830
Li	2.033746	1.123046	-2.405636
N	0.677875	1.793623	-1.136067
N	1.138425	2.882780	-0.680744
O	1.344313	2.911316	0.623986
C	-0.944437	0.215652	-0.141928
C	-1.279062	-1.032062	-0.739029
C	-2.003755	0.998207	0.403471
C	-2.608377	-1.487400	-0.711892
C	-3.317045	0.513710	0.388533
C	-3.645398	-0.737969	-0.149701
H	-2.840440	-2.455564	-1.167257
H	-4.111732	1.130395	0.821059
C	0.653027	-1.240327	2.117773
H	0.304046	-0.255867	2.472697
H	-0.233885	-1.745700	1.702202
H	1.003780	-1.824869	2.981771
C	-5.066923	-1.241644	-0.119921
H	-5.400866	-1.430209	0.915576
H	-5.764873	-0.502209	-0.547766
H	-5.179519	-2.180857	-0.682943
C	-1.743323	2.348737	1.021726
H	-0.999990	2.285352	1.832399
H	-1.344639	3.067402	0.288383
H	-2.666668	2.777606	1.439082
C	-0.258370	-1.901668	-1.437944
H	0.412605	-1.313986	-2.081694
H	0.387388	-2.445594	-0.729148
H	-0.757241	-2.652694	-2.068937

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TS_B6_mes-THF2 SCF Done: -1333.06019461 A.U.

C	0.104149	1.648399	-0.838077
C	0.845573	2.627831	-1.577912
C	0.273458	3.134669	-2.740886
C	-0.997364	2.714175	-3.167915
C	-1.656751	1.776805	-2.383218
N	-1.125782	1.251175	-1.270415
H	0.817341	3.890881	-3.315866
H	-1.457913	3.113148	-4.073851
H	-2.654846	1.416283	-2.659983
C	0.581714	1.104458	0.432717
H	0.090212	2.268569	1.313798
Li	-1.700329	-0.441955	-0.280502
N	-0.473052	0.357290	1.161476
N	-1.157406	1.076556	1.947659

O	-0.826391	2.356223	1.977432
C	1.918313	0.449536	0.575737
C	2.545658	-0.270017	-0.482625
C	2.579901	0.479996	1.839761
C	3.802030	-0.864816	-0.276536
C	3.821400	-0.147023	2.002720
C	4.464946	-0.815880	0.953242
H	4.266185	-1.406867	-1.106940
H	4.308527	-0.103855	2.982489
C	-3.924308	-1.453039	1.198259
O	-3.529946	-0.453682	0.230439
C	-4.185773	0.804211	0.511281
C	-4.742149	0.656519	1.922596
C	-5.090344	-0.836441	1.967692
H	-4.185251	-2.379308	0.662462
H	-3.068133	-1.661296	1.864394
H	-3.447383	1.612827	0.409128
H	-4.988931	0.959739	-0.231759
H	-3.953584	0.887318	2.656225
H	-5.602542	1.316229	2.107645
H	-5.174538	-1.237893	2.988257
H	-6.041191	-1.026111	1.442388
C	-0.113784	-2.893340	0.010156
O	-1.036420	-2.138939	-0.811091
C	-1.253955	-2.803763	-2.073390
C	-0.624855	-4.186634	-1.916415
C	0.521420	-3.905424	-0.936339
H	0.599567	-2.191981	0.464584
H	-0.682780	-3.390735	0.816005
H	-2.336126	-2.830885	-2.277221
H	-0.761127	-2.220422	-2.871543
H	-1.348054	-4.887850	-1.468167
H	-0.290910	-4.604208	-2.877559
H	0.878798	-4.802211	-0.409539
H	1.375882	-3.449449	-1.461748
C	2.178372	3.122652	-1.090115
H	2.965931	2.357992	-1.191417
H	2.498979	4.016872	-1.646075
H	2.131489	3.369415	-0.015945
C	1.898534	-0.468623	-1.834749
H	0.835317	-0.724635	-1.741938
H	1.952727	0.433668	-2.465236
H	2.397970	-1.280014	-2.385201
C	1.972920	1.186457	3.025709
H	1.696510	2.224004	2.782175
H	1.047033	0.694268	3.364887
H	2.671305	1.206354	3.875827
C	5.820596	-1.447292	1.151550
H	6.085835	-2.114907	0.317071
H	6.611396	-0.679415	1.225071
H	5.860798	-2.034116	2.084360
36			
B7 SCF Done: -903.652198015 A.U.			
C	-1.500441	-1.406079	-1.407806
C	-0.394415	-0.632672	-1.152003
C	-0.449980	0.356684	-0.129170
C	-2.670476	-0.189600	0.350672

C	-2.686168	-1.215813	-0.647126
H	-1.480875	-2.171299	-2.188685
H	0.530471	-0.765284	-1.714384
C	0.771321	1.230281	0.140990
H	0.636932	1.682947	1.138983
C	2.053518	0.408713	0.168593
C	3.039826	0.508495	-0.819109
C	2.255225	-0.501832	1.220298
C	4.194087	-0.282303	-0.757180
H	2.897510	1.214617	-1.637878
C	3.404684	-1.288738	1.277900
H	1.496182	-0.595811	2.003341
C	4.399862	-1.194213	0.287477
H	4.950760	-0.185234	-1.541675
H	3.537944	-1.989827	2.107717
N	-1.555897	0.576935	0.574191
N	0.171308	3.340582	-0.734549
N	0.851759	2.288693	-0.893691
O	-0.602765	3.463306	0.302119
Li	-1.601938	2.430540	1.296337
C	5.643879	-2.043093	0.368013
H	6.281180	-1.918183	-0.520417
H	6.246982	-1.780344	1.254413
H	5.392753	-3.113234	0.460144
C	-4.990070	-1.742558	-0.074685
C	-3.866163	-1.983170	-0.839583
C	-3.841567	0.035698	1.123264
C	-4.974900	-0.725226	0.912548
H	-5.895982	-2.334326	-0.227067
H	-3.866548	-2.764176	-1.604649
H	-3.829144	0.814760	1.890641
H	-5.869734	-0.543588	1.513344

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B7-THF2 SCF Done: -1368.81680917 A.U.

C	-0.218826	3.487086	-0.306319
C	-1.026075	2.458031	-0.724933
C	-0.591497	1.110357	-0.556174
C	1.399956	1.815936	0.422973
C	1.033795	3.195047	0.301265
H	-0.527412	4.529309	-0.426870
H	-1.997691	2.649196	-1.182787
C	-1.480692	-0.028291	-1.037750
H	-1.066423	-0.956178	-0.616353
C	-2.907449	0.120493	-0.529246
C	-3.985191	0.424034	-1.368809
C	-3.162973	-0.051169	0.842884
C	-5.279889	0.553786	-0.850734
H	-3.799465	0.551607	-2.435923
C	-4.453235	0.079045	1.355847
H	-2.334656	-0.288095	1.517048
C	-5.540547	0.384331	0.516506
H	-6.105562	0.791598	-1.528428
H	-4.624779	-0.061205	2.427704
N	0.586272	0.810197	-0.026770
N	-0.485561	-0.686131	-3.066694
N	-1.449865	-0.073559	-2.517599
O	0.439963	-1.221350	-2.339915

Li	1.261956	-1.063742	-0.710480
C	-6.934284	0.505840	1.080321
H	-7.647246	0.876848	0.328434
H	-7.303835	-0.470700	1.439231
H	-6.959579	1.192262	1.943195
C	3.120131	3.847301	1.369148
C	1.918943	4.196429	0.783843
C	2.641053	1.486208	1.032864
C	3.479708	2.481378	1.495213
H	3.796918	4.621610	1.739054
H	1.629866	5.246281	0.684044
H	2.912497	0.433753	1.116617
H	4.430716	2.214906	1.964145
C	4.124361	-0.469450	-1.412607
O	3.175478	-1.261410	-0.686025
C	3.920052	-2.260939	0.016225
C	5.145509	-1.511353	0.543733
C	5.390084	-0.420249	-0.530145
H	4.328334	-0.951785	-2.385606
H	3.670307	0.514515	-1.597871
H	3.266279	-2.685365	0.790145
H	4.210459	-3.067594	-0.684492
H	4.914222	-1.053448	1.518104
H	6.008142	-2.179230	0.682483
H	5.515134	0.570105	-0.069191
H	6.289201	-0.625724	-1.129292
C	0.248345	-2.062557	1.909929
O	0.664353	-2.405058	0.570643
C	-0.087920	-3.534564	0.084154
C	-1.354447	-3.549083	0.930867
C	-0.820953	-3.090737	2.295243
H	1.126481	-2.082482	2.576375
H	-0.144994	-1.032978	1.892768
H	-0.261338	-3.381742	-0.991365
H	0.505048	-4.457402	0.225388
H	-2.083519	-2.822518	0.536876
H	-1.833614	-4.538685	0.958818
H	-1.597103	-2.658338	2.943812
H	-0.364264	-3.939763	2.829417
36			
TS_B7 SCF Done: -903.603355117 A.U.			
C	-1.554287	-2.056105	-0.033591
C	-0.415361	-1.301847	-0.006634
C	-0.488068	0.138444	0.002058
C	-2.847830	0.003013	-0.058929
C	-2.835284	-1.426530	-0.061278
H	-1.495123	-3.148093	-0.056849
H	0.559166	-1.786548	-0.019426
C	0.733598	0.944638	0.017857
H	0.347109	1.859555	1.129210
C	2.077009	0.293836	-0.018697
C	2.978506	0.485721	-1.081973
C	2.509940	-0.507732	1.058068
C	4.242599	-0.112024	-1.074760
H	2.683700	1.113205	-1.925319
C	3.766880	-1.112215	1.054264
H	1.845029	-0.653932	1.914028

C	4.663854	-0.926031	-0.012579
H	4.916307	0.056595	-1.920665
H	4.066237	-1.731867	1.905633
N	-1.695651	0.747011	-0.003159
N	0.238168	3.163444	-0.232838
N	0.692276	2.159514	-0.801825
O	-0.149253	2.923060	1.087802
Li	-1.936819	2.552519	0.737424
C	6.031126	-1.562741	0.008922
H	6.662630	-1.125252	0.802152
H	5.968097	-2.644762	0.213761
H	6.557973	-1.428025	-0.948099
C	-5.267932	-1.477258	-0.135869
C	-4.055011	-2.144474	-0.100075
C	-4.107883	0.660606	-0.108206
C	-5.287678	-0.063955	-0.141051
H	-6.206183	-2.036415	-0.166375
H	-4.020002	-3.237702	-0.102279
H	-4.145089	1.754933	-0.140345
H	-6.243986	0.464406	-0.180507

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TS_B7-THF2 SCF Done: -1368.77775688 A.U.

C	-0.624618	3.674678	0.223655
C	0.352663	2.846856	0.706488
C	0.115975	1.430671	0.806759
C	-2.052077	1.718844	-0.052545
C	-1.883248	3.134526	-0.183007
H	-0.460087	4.754191	0.158076
H	1.307061	3.248514	1.050476
C	1.126262	0.544151	1.381707
H	1.329267	0.570431	2.859779
C	2.506523	0.501048	0.827342
C	3.461638	-0.396667	1.363813
C	2.927497	1.269186	-0.281704
H	3.194691	-1.019979	2.219204
C	4.219066	1.160120	-0.803557
H	2.228373	1.947660	-0.772923
C	5.159812	0.268666	-0.266023
H	4.492857	1.772671	-1.668716
N	-1.059911	0.910786	0.424107
N	0.656995	-1.151467	2.859795
N	0.566064	-0.802959	1.651850
O	1.246879	-0.275458	3.651492
Li	-0.870623	-1.130033	0.298117
C	-4.138259	3.334762	-1.079416
C	-2.944041	3.921779	-0.695827
C	-3.287589	1.142322	-0.456156
C	-4.304474	1.934247	-0.959453
H	-4.951581	3.947955	-1.475535
H	-2.800777	5.002590	-0.785531
H	-3.408086	0.062193	-0.362051
H	-5.247280	1.473096	-1.266922
C	4.743582	-0.510456	0.827310
H	5.443030	-1.225221	1.272974
C	6.559422	0.161370	-0.817717
H	6.618957	0.538156	-1.850994
H	7.275394	0.748723	-0.214427

H	6.918234	-0.880844	-0.813459
C	-3.403982	-2.107693	1.541548
O	-2.413250	-2.215069	0.507100
C	-2.931352	-3.118944	-0.476740
C	-4.407079	-2.734828	-0.594858
C	-4.767834	-2.242097	0.830099
H	-3.248343	-2.919761	2.274060
H	-3.254711	-1.144144	2.049901
H	-2.345176	-2.985892	-1.396692
H	-2.809552	-4.160073	-0.121328
H	-4.523424	-1.922206	-1.328413
H	-5.027161	-3.580231	-0.926680
H	-5.297614	-1.279146	0.795820
H	-5.412222	-2.957397	1.361615
C	1.032134	-2.630441	-1.265193
O	0.003073	-1.619200	-1.349038
C	0.349952	-0.631067	-2.346105
C	1.560247	-1.199567	-3.084356
C	2.234706	-2.040986	-1.993513
H	1.223602	-2.843259	-0.202329
H	0.667311	-3.551917	-1.754446
H	-0.525846	-0.461556	-2.992181
H	0.596642	0.314202	-1.835957
H	1.237655	-1.839819	-3.922181
H	2.209161	-0.406872	-3.485023
H	2.906367	-2.816815	-2.389496
H	2.809937	-1.394718	-1.312973

36

B8 SCF Done: -1201.51677079 A.U.

C	-2.069719	-1.662068	-1.038873
C	-1.003261	-0.852070	-0.731179
C	-1.215060	0.324021	0.042700
C	-3.505583	-0.113955	0.177299
C	-3.370696	-1.321263	-0.579769
H	-1.930433	-2.569737	-1.632355
H	0.004906	-1.096797	-1.067244
C	-0.037971	1.241365	0.362774
H	-0.333628	1.872446	1.218584
C	1.194467	0.447236	0.772560
C	2.317377	0.339835	-0.051923
C	1.197936	-0.216080	2.011895
C	3.419168	-0.425303	0.355425
H	2.322418	0.859729	-1.010202
C	2.297056	-0.974252	2.415860
H	0.324200	-0.136659	2.665364
C	3.417978	-1.085740	1.586159
H	2.285239	-1.482104	3.383326
N	-2.425416	0.681417	0.458793
N	-0.398064	3.145938	-0.986145
N	0.264056	2.083628	-0.818573
O	-1.341411	3.460203	-0.151341
Li	-2.566265	2.638703	0.787587
C	-5.761272	-1.717361	-0.379458
C	-4.522287	-2.110268	-0.844579
C	-4.792962	0.265545	0.643611
C	-5.894806	-0.520584	0.369174
H	-6.644665	-2.326184	-0.586803

H	-4.407553	-3.030378	-1.423689
H	-4.895253	1.184627	1.227557
H	-6.880381	-0.219789	0.733596
H	4.281080	-1.677577	1.894732
C	4.595846	-0.524172	-0.577873
F	5.099251	0.690634	-0.882024
F	5.605811	-1.253002	-0.068422
F	4.253033	-1.095578	-1.753580
62			
B8-THF2 SCF Done: -1666.68135176 A.U.			
C	-0.284729	3.475410	0.010233
C	0.542606	2.419128	0.303767
C	0.042248	1.087786	0.204518
C	-2.050208	1.860239	-0.461319
C	-1.624134	3.226183	-0.398467
H	0.072374	4.506522	0.081597
H	1.577091	2.576752	0.612945
C	0.957375	-0.076974	0.556459
H	0.454869	-0.999756	0.224345
C	2.287963	0.016714	-0.177253
C	3.507117	0.081185	0.502126
C	2.297676	0.016432	-1.583703
C	4.711022	0.145673	-0.213333
H	3.502440	0.075559	1.592290
C	3.497190	0.079084	-2.293521
H	1.349941	-0.033953	-2.126688
C	4.716281	0.145477	-1.610424
H	3.486453	0.073775	-3.386283
N	-1.210164	0.827015	-0.140986
N	0.276092	-0.650302	2.733310
N	1.171198	-0.103661	2.020076
O	-0.782793	-1.135672	2.179094
Li	-1.840515	-0.999335	0.687652
C	-3.827787	3.950317	-1.131350
C	-2.539889	4.257900	-0.739288
C	-3.381099	1.573230	-0.870296
C	-4.247610	2.597386	-1.198297
H	-4.527830	4.747917	-1.392246
H	-2.204781	5.297313	-0.685565
H	-3.697918	0.530733	-0.908218
H	-5.268561	2.364308	-1.512276
H	5.658759	0.192862	-2.158343
C	5.996953	0.250881	0.561581
F	6.055161	-0.648085	1.565596
F	7.084681	0.055692	-0.207639
F	6.138838	1.467345	1.134363
C	-4.526362	-0.288306	1.829616
O	-3.736251	-1.125262	0.974539
C	-4.621087	-2.096573	0.408556
C	-5.882981	-1.299615	0.070895
C	-5.913839	-0.195777	1.158778
H	-4.591155	-0.752091	2.830418
H	-4.011024	0.678180	1.924648
H	-4.115184	-2.549316	-0.454941
H	-4.829938	-2.887559	1.154745
H	-5.786968	-0.854793	-0.931751
H	-6.782820	-1.931850	0.073678

H	-6.075098	0.796573	0.713692
H	-6.712862	-0.365229	1.895301
C	-1.072978	-2.196901	-1.961597
O	-1.506647	-2.412039	-0.605959
C	-0.982070	-3.662681	-0.101159
C	-0.258358	-4.315185	-1.281091
C	0.140375	-3.102949	-2.132852
H	-1.887277	-2.477373	-2.655487
H	-0.862637	-1.124175	-2.086811
H	-0.301327	-3.433003	0.735463
H	-1.817593	-4.267254	0.287129
H	0.598601	-4.923546	-0.957052
H	-0.947146	-4.965713	-1.844754
H	1.038168	-2.616908	-1.717216
H	0.338430	-3.350501	-3.186137
36			
TS_B8 SCF Done: -1201.46884196 A.U.			
C	-2.467103	-2.047413	0.090184
C	-1.302395	-1.360337	0.290545
C	-1.283219	0.079576	0.243876
C	-3.597088	0.080360	-0.233602
C	-3.678729	-1.345796	-0.183504
H	-2.475692	-3.140951	0.112647
H	-0.374829	-1.904574	0.457998
C	-0.033644	0.822916	0.440821
H	-0.536120	1.826632	1.415580
C	1.249955	0.108466	0.681145
C	2.360478	0.271331	-0.168276
C	1.411148	-0.711404	1.818617
C	3.567673	-0.380534	0.101418
H	2.277693	0.917454	-1.042508
C	2.614992	-1.368018	2.077154
H	0.577108	-0.823466	2.516007
C	3.707320	-1.209942	1.219903
H	2.709056	-1.996309	2.966598
N	-2.427305	0.756918	0.007370
N	-0.335889	3.042710	-0.013971
N	0.140340	1.981706	-0.443546
O	-0.947489	2.910880	1.232832
Li	-2.692109	2.602664	0.656918
C	-6.056508	-1.255166	-0.694484
C	-4.917943	-1.991274	-0.415053
C	-4.779200	0.809052	-0.538762
C	-5.979657	0.155107	-0.758627
H	-7.009999	-1.758002	-0.873117
H	-4.956636	-3.083404	-0.370956
H	-4.734183	1.900143	-0.622598
H	-6.875458	0.735946	-0.993871
H	4.656217	-1.708770	1.424519
C	4.711649	-0.231707	-0.865079
F	5.909209	-0.407332	-0.271745
F	4.733652	0.981365	-1.451152
F	4.645215	-1.138517	-1.867140
62			
TS_B8-THF2 SCF Done: -1666.64446579 A.U.			
C	2.042342	-3.646843	0.289012

C	0.860451	-3.082710	0.694534
C	0.730161	-1.654590	0.755908
C	2.943274	-1.399070	0.023006
C	3.142529	-2.813757	-0.070587
H	2.159583	-4.733708	0.251590
H	0.019193	-3.704676	1.004751
C	-0.517700	-1.030384	1.228352
H	-0.960537	-1.190305	2.633533
C	-1.773414	-1.223351	0.469470
C	-2.900083	-0.417186	0.759466
C	-1.919236	-2.152281	-0.591039
C	-4.083086	-0.532263	0.028306
H	-2.850850	0.323734	1.556838
C	-3.115848	-2.279019	-1.297265
H	-1.076213	-2.776842	-0.887713
C	-4.215700	-1.467830	-1.004541
H	-3.182704	-3.010482	-2.107259
N	1.754429	-0.861348	0.424685
N	-0.649053	0.625402	2.811459
N	-0.282603	0.375125	1.630039
O	-1.195298	-0.388516	3.450382
Li	1.093995	1.090926	0.381117
C	5.420950	-2.451118	-0.846098
C	4.396258	-3.315660	-0.504875
C	4.012906	-0.533788	-0.336414
C	5.222014	-1.050948	-0.763077
H	6.383877	-2.844024	-1.181847
H	4.536809	-4.398574	-0.567195
H	3.850136	0.542769	-0.271176
H	6.034245	-0.372598	-1.038573
H	-5.145185	-1.547513	-1.569970
C	-5.179267	0.464153	0.279843
F	-4.960369	1.615514	-0.405284
F	-5.279985	0.812540	1.577664
F	-6.389470	0.016421	-0.106144
C	3.347013	2.580374	1.689560
O	2.356894	2.484321	0.653470
C	2.651042	3.511730	-0.301765
C	4.175201	3.480502	-0.423933
C	4.642384	3.043752	0.988355
H	3.009829	3.315299	2.442183
H	3.424518	1.595219	2.171820
H	2.108769	3.273819	-1.227425
H	2.293646	4.485982	0.082890
H	4.473615	2.737592	-1.179650
H	4.583764	4.454729	-0.729199
H	5.378630	2.229073	0.929788
H	5.106783	3.872385	1.542430
C	0.247364	0.474664	-2.387305
O	0.189062	1.408683	-1.287716
C	-1.063128	2.132491	-1.306927
C	-1.926356	1.424269	-2.346886
C	-0.874915	0.896352	-3.330734
H	1.252569	0.524778	-2.834305
H	0.084753	-0.545946	-2.000875
H	-1.496723	2.113698	-0.295417
H	-0.858024	3.181294	-1.586713
H	-2.466792	0.587176	-1.881770

H	-2.665230	2.097826	-2.804896
H	-1.235357	0.059927	-3.947581
H	-0.532254	1.701222	-4.002292
26			
B9 SCF Done: -726.655889609 A.U.			
C	-1.823843	-2.278785	-1.075357
C	-0.835149	-1.311500	-0.911459
C	-1.030082	-0.276065	0.015365
C	-3.120023	-1.123582	0.572199
C	-2.991540	-2.192814	-0.310636
H	-1.685365	-3.093812	-1.790418
H	0.089853	-1.353678	-1.488609
H	-4.025302	-1.007981	1.177234
H	-3.790066	-2.931988	-0.399794
C	0.017164	0.815892	0.198842
H	-0.126819	1.246265	1.205486
C	1.428436	0.244542	0.165954
C	2.384032	0.633474	-0.781249
C	3.655262	0.055381	-0.727864
H	2.117871	1.372775	-1.535900
C	2.908214	-1.209255	1.165436
C	3.929257	-0.887872	0.264044
H	4.420980	0.338990	-1.455063
H	3.086847	-1.944462	1.959497
N	-2.170956	-0.184944	0.728930
N	-0.971490	2.789928	-0.639527
N	-0.145388	1.855868	-0.840939
O	-1.681350	2.804701	0.448562
Li	-2.501618	1.629348	1.452308
H	4.908417	-1.365701	0.343903
N	1.691958	-0.661216	1.121051
2			
B9-THF2 SCF Done: -1191.81991469 A.U.			
C	1.741751	3.651714	-1.116691
C	2.053805	2.542570	-0.332825
C	1.086831	1.543493	-0.141096
C	-0.437307	2.712156	-1.439232
C	0.469219	3.741372	-1.689909
H	2.482603	4.438873	-1.279826
H	3.037867	2.440892	0.128327
H	-1.449733	2.745851	-1.855671
H	0.181517	4.590590	-2.313164
C	1.363493	0.339609	0.748975
H	0.643753	-0.443303	0.471252
C	2.749101	-0.234123	0.505021
C	3.770986	-0.189990	1.462245
C	5.013666	-0.744775	1.145999
H	3.572246	0.272143	2.428796
C	4.115020	-1.323926	-0.998700
C	5.196036	-1.325570	-0.110714
H	5.829482	-0.722761	1.873818
H	4.217969	-1.773853	-1.993407
H	6.149536	-1.772774	-0.401060
N	-0.140333	1.643839	-0.685463
N	0.023217	0.649256	2.659549
N	1.189065	0.721982	2.168101

O	-0.972540	0.280864	1.919590
Li	-1.486430	0.349448	0.133133
C	-1.309835	-2.534618	0.171538
O	-1.270642	-1.399236	-0.716827
C	-0.442510	-1.686658	-1.868064
C	-0.040475	-3.156802	-1.732597
C	-0.096500	-3.372570	-0.214317
H	-1.287067	-2.154211	1.203800
H	-2.253088	-3.089895	0.012058
H	-1.018588	-1.471504	-2.782387
H	0.440525	-1.028362	-1.837988
H	-0.771000	-3.809795	-2.238090
H	0.952731	-3.351546	-2.163165
H	-0.201432	-4.428234	0.076543
H	0.811119	-2.968243	0.262855
C	-4.087648	0.723453	1.287439
O	-3.380930	0.712975	0.029267
C	-4.190295	0.076745	-0.985743
C	-5.476232	-0.377441	-0.281904
C	-5.044701	-0.456498	1.189037
H	-3.336299	0.643164	2.085915
H	-4.636148	1.678469	1.394972
H	-4.379584	0.793961	-1.801861
H	-3.613322	-0.770660	-1.390015
H	-6.269735	0.378057	-0.401826
H	-5.852954	-1.330991	-0.680550
H	-5.884358	-0.385687	1.896333
H	-4.501463	-1.396238	1.385986
N	2.925362	-0.794784	-0.703341

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TS_B9 SCF Done: -726.606826343 A.U.

C	-1.146356	-0.266256	-0.056756
C	-1.116311	-1.680774	-0.171294
C	-2.297818	-2.401177	-0.251265
C	-3.530033	-1.729738	-0.212777
C	-3.493776	-0.349290	-0.081921
N	-2.356321	0.367101	0.005167
H	-2.262537	-3.489062	-0.357845
H	-0.154682	-2.186457	-0.194152
H	-4.482023	-2.259274	-0.279720
H	-4.428071	0.223209	-0.035438
C	0.073709	0.567826	-0.021879
H	-0.300239	1.498378	1.093098
Li	-2.602167	2.163579	0.770961
N	-0.021355	1.779704	-0.856952
N	-0.470953	2.779924	-0.278286
O	-0.797760	2.552028	1.059669
C	1.438837	0.006405	-0.024441
C	2.515108	0.715090	-0.619281
C	2.909833	-1.634828	0.699716
C	3.803998	0.200440	-0.538508
H	2.326382	1.656959	-1.135085
C	4.022586	-1.006165	0.138446
H	3.031161	-2.581756	1.241410
H	4.636831	0.738448	-1.000496
N	1.666328	-1.154377	0.628073
H	5.019206	-1.443074	0.231738

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TS_B9-THF2 SCF Done: -1191.77891852 A.U.

C	0.907142	1.914006	0.199596
C	1.817648	2.995263	0.145117
C	1.499980	4.132087	-0.588387
C	0.266453	4.200823	-1.252278
C	-0.589138	3.108426	-1.137769
N	-0.283988	1.999776	-0.448443
H	2.199576	4.971666	-0.629388
H	2.753272	2.937259	0.703900
H	-0.026570	5.079040	-1.830895
H	-1.568611	3.116461	-1.629685
C	1.181874	0.690504	0.979283
H	1.263194	0.749040	2.431808
Li	-1.299616	0.225498	-0.305841
N	-0.058007	-0.074921	1.227424
N	-0.266268	-0.292113	2.454918
O	0.645716	0.174377	3.268070
C	2.348858	-0.158308	0.668379
C	3.392434	0.221272	-0.217012
C	4.461883	-0.640514	-0.431497
H	3.353660	1.173619	-0.745176
C	3.417332	-2.184018	1.058180
C	4.494233	-1.879445	0.223058
H	5.263506	-0.352616	-1.118105
H	3.386049	-3.151045	1.577387
H	5.315160	-2.586021	0.083533
C	-4.193528	-0.248811	-0.882757
O	-3.148347	0.017970	0.077446
C	-3.660140	-0.085453	1.425695
C	-4.964613	-0.859805	1.286168
C	-5.481682	-0.352824	-0.066229
H	-4.210125	0.561996	-1.628560
H	-3.961931	-1.194650	-1.403038
H	-2.898882	-0.577246	2.048306
H	-3.834065	0.931081	1.823622
H	-4.761693	-1.942882	1.241030
H	-5.656669	-0.671802	2.120073
H	-6.219374	-1.020283	-0.535248
H	-5.943367	0.641328	0.051964
C	-1.178398	-2.379547	-1.378839
O	-0.886927	-1.016219	-1.726418
C	0.410074	-0.967238	-2.360471
C	1.108449	-2.305571	-2.042588
C	0.176871	-2.970113	-1.013183
H	-1.905804	-2.370061	-0.553644
H	-1.632754	-2.897565	-2.245595
H	0.276855	-0.815754	-3.445608
H	0.946816	-0.097597	-1.954222
H	1.186865	-2.922206	-2.951569
H	2.122591	-2.152664	-1.647148
H	0.189412	-4.069006	-1.064552
H	0.450623	-2.659833	0.006164
N	2.384431	-1.368481	1.276469

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B10 SCF Done: -881.563657173 A.U.

C	2.530682	-2.398254	1.270762
C	1.708330	-1.313693	0.973983
C	2.112870	-0.383957	0.003246
C	4.084217	-1.567018	-0.348195
C	3.744395	-2.538194	0.590156
H	2.226676	-3.130712	2.023022
H	0.750149	-1.182184	1.478208
H	5.031102	-1.629395	-0.894943
H	4.416939	-3.376143	0.783729
C	1.254771	0.833533	-0.330408
H	1.522949	1.147502	-1.353703
N	3.297711	-0.514823	-0.632040
N	2.523222	2.703642	0.379275
N	1.564138	1.923180	0.629895
O	3.247716	2.528171	-0.688614
Li	3.944494	1.145728	-1.496127
C	-2.936779	-0.194331	-0.383709
C	-2.435042	0.584151	0.702039
C	-1.069312	0.932808	0.725497
C	-0.234483	0.513241	-0.309448
C	-0.763734	-0.258196	-1.377485
C	-2.105930	-0.621056	-1.431446
C	-4.645673	0.228678	0.997960
C	-3.551344	0.839209	1.570676
H	-0.656282	1.532478	1.537295
H	-0.093220	-0.575814	-2.181691
H	-2.497764	-1.211204	-2.262926
H	-5.679417	0.185629	1.339428
H	-3.544692	1.404451	2.501120
N	-4.284884	-0.395901	-0.178770
C	-5.160514	-1.133093	-1.065153
H	-5.187317	-0.670526	-2.065550
H	-4.822165	-2.176722	-1.173320
H	-6.178212	-1.135561	-0.652746

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B10-THF2 SCF Done: -1346.72711643 A.U.

C	-0.183943	-3.729829	-1.543745
C	-0.705417	-2.775310	-0.672945
C	0.058751	-1.639414	-0.360516
C	1.788660	-2.382884	-1.715756
C	1.090992	-3.531795	-2.085099
H	-0.764835	-4.619975	-1.799681
H	-1.698184	-2.893840	-0.235706
H	2.796002	-2.191823	-2.101016
H	1.537987	-4.251877	-2.773679
C	-0.444404	-0.595523	0.628453
H	0.145711	0.316410	0.454041
N	1.290202	-1.462530	-0.877194
N	0.916652	-0.895859	2.539087
N	-0.213436	-1.097803	2.006086
O	1.852606	-0.288178	1.880180
Li	2.415977	-0.088299	0.132699
C	-4.571667	0.420278	-0.126564
C	-4.252226	-0.324414	1.048038
C	-2.906878	-0.658099	1.307187
C	-1.913612	-0.255836	0.415925
C	-2.263091	0.488518	-0.742585

C	-3.580128	0.833855	-1.029929
C	-6.483186	0.020706	0.966851
C	-5.495351	-0.565384	1.728013
H	-2.626488	-1.220548	2.198317
H	-1.470219	0.796966	-1.429510
H	-3.829981	1.409209	-1.924203
H	-7.559074	0.064449	1.133285
H	-5.639484	-1.104551	2.662818
N	-5.936196	0.615952	-0.151720
C	-6.655712	1.331223	-1.184098
H	-6.324978	2.381532	-1.240029
H	-6.496498	0.863201	-2.169451
H	-7.729977	1.313197	-0.957689
C	5.130023	0.565651	-0.819293
O	4.326092	-0.314276	-0.002852
C	5.018730	-0.629942	1.224789
C	6.044536	0.484844	1.384629
C	6.455887	0.735063	-0.072238
H	5.250412	0.118238	-1.819768
H	4.588504	1.520362	-0.927387
H	4.266170	-0.678694	2.025265
H	5.508274	-1.616650	1.123866
H	5.564404	1.381669	1.811016
H	6.884332	0.198827	2.035107
H	6.904483	1.725434	-0.239771
H	7.182000	-0.028330	-0.396883
C	1.359955	2.009524	-1.735555
O	2.042712	1.721921	-0.497175
C	1.714222	2.712380	0.497419
C	0.374511	3.280078	0.046169
C	0.532039	3.275789	-1.481050
H	2.105100	2.138316	-2.537990
H	0.731884	1.139359	-1.988078
H	1.688536	2.205571	1.473125
H	2.499912	3.490991	0.512859
H	-0.444874	2.610318	0.353258
H	0.177071	4.279509	0.460869
H	-0.428856	3.256823	-2.016092
H	1.086736	4.169882	-1.808620
34			
TS_B10 SCF Done: -881.511663401 A.U.			
C	2.183182	0.348821	-0.068736
C	1.763863	1.704686	-0.204143
C	2.690879	2.707390	-0.425634
C	4.057691	2.387242	-0.520410
C	4.404408	1.052774	-0.377604
N	3.520009	0.060615	-0.150818
H	2.354625	3.741522	-0.543229
H	0.702830	1.944950	-0.155454
H	4.820059	3.146516	-0.702696
H	5.457127	0.750375	-0.440494
C	1.217943	-0.732229	0.159009
H	1.965274	-1.410634	1.301400
Li	4.297308	-1.571409	0.600957
N	1.492131	-1.980525	-0.547712
N	2.258791	-2.769283	0.027306
O	2.717908	-2.287113	1.266427

C	-2.975873	0.228297	0.306517
C	-2.475864	-0.520254	-0.800469
C	-1.102433	-0.827675	-0.860151
C	-0.245461	-0.409610	0.165276
C	-0.785852	0.316789	1.264199
C	-2.134262	0.651994	1.346062
C	-4.700662	-0.211637	-1.050536
C	-3.603095	-0.787543	-1.652703
H	-0.704169	-1.397527	-1.702121
H	-0.111606	0.618761	2.070255
H	-2.523155	1.213261	2.198852
H	-5.741066	-0.186912	-1.373252
H	-3.600887	-1.335828	-2.593366
N	-4.333120	0.402037	0.129335
C	-5.208738	1.102882	1.043938
H	-5.215354	0.617301	2.033919
H	-4.886158	2.149277	1.172702
H	-6.231745	1.098601	0.644724

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TS_B10-THF2 SCF Done: -1346.68081850 A.U.

C	0.182320	1.567584	-0.852752
C	1.102462	2.505217	-1.400154
C	0.655224	3.495088	-2.259850
C	-0.708708	3.562831	-2.598011
C	-1.548017	2.601029	-2.047571
N	-1.133602	1.636919	-1.211161
H	1.364250	4.217073	-2.675562
H	2.158070	2.439440	-1.135425
H	-1.100318	4.329356	-3.269429
H	-2.617637	2.596926	-2.290691
C	0.571021	0.540393	0.107083
H	0.482487	0.588262	1.580199
Li	-2.223905	0.071474	-0.561245
N	-0.432124	-0.513177	0.229787
N	-0.600219	-0.906635	1.426366
O	0.134354	-0.265198	2.317261
C	4.621520	-0.940159	-0.071560
C	4.348166	0.252048	0.663878
C	3.020902	0.718186	0.738145
C	1.996443	0.034087	0.075816
C	2.308912	-1.150829	-0.647085
C	3.605300	-1.652535	-0.725981
C	6.558273	-0.203883	0.776537
C	5.606823	0.699984	1.196271
H	2.786319	1.616541	1.316474
H	1.499047	-1.679655	-1.155507
H	3.823264	-2.565361	-1.285483
H	7.631545	-0.224662	0.963314
H	5.785227	1.579937	1.812155
N	5.974527	-1.194441	0.013361
C	6.649226	-2.317605	-0.601360
H	6.252970	-3.272564	-0.218380
H	6.520712	-2.302344	-1.696240
H	7.722305	-2.266762	-0.373628
C	-2.954300	1.891803	1.582429
O	-3.313175	0.650419	0.933491
C	-3.742334	-0.319331	1.914447

C	-3.325763	0.261247	3.262381
C	-3.474289	1.766781	3.011532
H	-1.856572	2.001988	1.562249
H	-3.398123	2.725453	1.016449
H	-4.838589	-0.440286	1.841371
H	-3.259995	-1.282282	1.692619
H	-3.944180	-0.112999	4.091556
H	-2.271406	0.014038	3.463292
H	-4.534608	2.065517	3.065572
H	-2.903998	2.388614	3.717330
C	-2.898987	-2.668815	-1.216430
O	-3.251644	-1.283913	-1.423824
C	-4.681670	-1.151490	-1.595256
C	-5.240543	-2.576747	-1.561880
C	-4.186356	-3.325952	-0.736299
H	-2.554525	-3.104304	-2.172475
H	-2.069737	-2.707320	-0.494927
H	-5.070006	-0.532512	-0.768821
H	-4.882398	-0.629511	-2.544874
H	-6.249694	-2.616861	-1.126337
H	-5.290978	-2.994092	-2.580768
H	-4.329550	-3.135294	0.340111
H	-4.192266	-4.413484	-0.900274

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A0' SCF Done: -515.126785437 A.U.

C	-0.718609	0.069981	0.612893
C	-1.116393	-1.141033	0.021308
C	-2.332898	-1.192361	-0.657909
C	-3.115667	-0.035787	-0.723624
C	-2.636182	1.119864	-0.102403
N	-1.468018	1.177204	0.548308
H	-2.666508	-2.121181	-1.128169
H	-0.472395	-2.020185	0.095949
H	-4.076263	-0.026496	-1.243664
H	-3.223844	2.045119	-0.132432
C	0.601092	0.163854	1.360137
C	1.756727	-0.221670	0.458396
O	2.230836	-1.332130	0.378858
H	0.724888	1.193241	1.719598
O	2.163108	0.813643	-0.288504
C	3.201991	0.550344	-1.240194
H	2.882047	-0.212346	-1.967345
H	3.396264	1.500971	-1.753139
H	4.116310	0.199290	-0.737039
H	0.603711	-0.530096	2.213626

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TS_A0A' SCF Done: -1347.96250032 A.U.

C	-1.638880	0.344429	-0.288489
C	-2.303799	1.248109	0.569577
C	-3.499645	0.874751	1.177286
C	-4.030968	-0.395818	0.932460
C	-3.312745	-1.235827	0.082110
N	-2.158026	-0.892646	-0.502802
H	-4.018488	1.576608	1.836555
H	-1.875585	2.232452	0.744579
H	-4.967504	-0.728185	1.385101

H	-3.686827	-2.244464	-0.134775
C	-0.354400	0.602789	-0.989210
C	0.343918	1.897550	-1.022073
O	1.073790	2.262243	-1.927417
H	0.491282	-0.207637	-0.455942
O	0.220025	2.635077	0.115937
C	0.995379	3.831015	0.186999
H	0.758154	4.511928	-0.645403
H	0.739959	4.306619	1.143578
H	2.073659	3.607228	0.159453
H	-0.387340	0.211356	-2.016175
C	2.420163	-0.838444	0.685121
C	3.372665	-0.112679	-0.289961
H	3.658869	-0.794743	-1.108485
H	2.871839	0.756404	-0.745123
H	4.295502	0.238753	0.203813
C	3.133890	-2.076895	1.260696
H	2.464005	-2.609507	1.956800
H	3.402785	-2.771816	0.446914
H	4.057561	-1.815249	1.805968
C	2.044749	0.111831	1.843235
H	1.537030	1.008960	1.456576
H	1.346346	-0.396686	2.528800
H	2.925913	0.436915	2.423232
O	1.270357	-1.255924	0.012650
K	-0.216648	-2.931918	-0.945354

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A' SCF Done: -1114.42553521 A.U.

C	-1.170604	-0.169892	0.299225
C	-1.746121	0.989341	-0.304478
C	-3.101079	1.011571	-0.606043
C	-3.901800	-0.103144	-0.313094
C	-3.265668	-1.196391	0.281735
N	-1.967823	-1.244940	0.578001
H	-3.539239	1.901689	-1.068909
H	-1.112332	1.847240	-0.519617
H	-4.971511	-0.123951	-0.532985
H	-3.851005	-2.092241	0.533170
C	0.218826	-0.328196	0.643967
C	1.318602	0.545212	0.502551
O	2.512494	0.233220	0.740629
H	0.436170	-1.259535	1.177564
K	2.518509	-1.944008	-0.572920
O	1.050497	1.803888	0.032826
C	2.165501	2.652839	-0.195568
H	2.845286	2.242569	-0.962144
H	1.756527	3.610264	-0.549208
H	2.749315	2.819806	0.724188

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TS_AB' SCF Done: -1298.94258148 A.U.

C	-1.612321	-0.182259	-0.303212
C	-2.448822	0.772183	0.329801
C	-3.824445	0.566933	0.355227
C	-4.362253	-0.583308	-0.234969
C	-3.466002	-1.480677	-0.823003
N	-2.146152	-1.298763	-0.861480

H	-4.476756	1.299129	0.840466
H	-2.007624	1.652927	0.791554
H	-5.436141	-0.783322	-0.235320
H	-3.842888	-2.400202	-1.290269
C	-0.158550	-0.106786	-0.361630
C	0.681506	1.058775	-0.302044
O	1.885759	1.065842	-0.611655
K	3.683324	-0.737314	-0.707076
H	0.292048	-0.929806	-0.920541
N	0.278409	-0.842091	1.642200
N	1.204159	-1.561431	1.603188
O	2.050860	-2.026656	0.817682
O	0.100866	2.188452	0.159893
C	0.930298	3.341702	0.284104
H	1.753123	3.167001	0.996131
H	1.361953	3.633376	-0.686358
H	0.281883	4.145368	0.658438

23

B' SCF Done: -1298.97048645 A.U.

C	-1.617729	-0.462302	-0.065012
C	-2.433530	-0.017724	0.986362
C	-3.783334	0.223332	0.731022
C	-4.274044	0.014623	-0.561409
C	-3.381654	-0.428203	-1.541532
N	-2.085996	-0.660651	-1.305092
H	-4.445077	0.568645	1.530046
H	-2.002287	0.121057	1.977914
H	-5.324320	0.187983	-0.807418
H	-3.731984	-0.605769	-2.565493
C	-0.130882	-0.701359	0.136652
C	0.631318	0.579623	-0.200168
K	3.564909	-0.461194	-1.005258
H	0.201108	-1.437578	-0.613966
N	0.123383	-1.196095	1.505285
N	1.339308	-1.306703	1.829942
O	2.234240	-0.941009	0.974631
O	1.252094	0.783956	-1.233294
O	0.445677	1.518173	0.728719
C	1.102843	2.773622	0.532809
H	0.772117	3.423524	1.353000
H	2.197437	2.652420	0.578134
H	0.828850	3.217897	-0.436063

23

TS_BC' SCF Done: -1298.93804864 A.U.

C	1.593279	-0.154987	-0.054820
C	2.442324	0.969443	0.075910
C	3.821378	0.781075	0.126372
C	4.346998	-0.512540	0.044144
C	3.436843	-1.564378	-0.083536
N	2.114189	-1.401126	-0.125534
H	4.484274	1.645679	0.224968
H	2.019469	1.968911	0.131393
H	5.422170	-0.702324	0.079150
H	3.800147	-2.598310	-0.150078
C	0.112539	-0.119031	-0.082817
C	-0.731094	1.064607	-0.182542

O	-1.946743	1.013543	-0.410155
K	-3.769402	-0.769234	-0.008544
H	-0.505609	-0.698848	1.034765
N	-0.464479	-1.253660	-0.855905
N	-1.205122	-1.979389	-0.153012
O	-1.340420	-1.610757	1.127596
O	-0.139839	2.242225	0.089899
C	-0.980547	3.397675	0.135568
H	-1.742962	3.302546	0.924956
H	-0.318646	4.244899	0.358276
H	-1.486624	3.560862	-0.828322
23			
C1 SCF Done: -1298.96298824 A.U.			
C	-1.513950	-0.129979	0.267222
C	-1.930696	1.130969	-0.203758
C	-3.234082	1.264283	-0.678706
C	-4.086078	0.155764	-0.678477
C	-3.578030	-1.053492	-0.195013
N	-2.334776	-1.198546	0.264848
H	-3.580531	2.232341	-1.050524
H	-1.243732	1.973276	-0.191475
H	-5.113628	0.221842	-1.042324
H	-4.210142	-1.949708	-0.179086
C	-0.152463	-0.387804	0.762396
C	1.031489	0.500465	0.859106
O	2.151887	0.064785	1.112961
K	3.006734	-0.943724	-1.191520
H	0.455798	1.059629	-1.796982
N	0.155869	-1.647130	0.962724
N	0.478024	-2.724253	1.113500
O	1.233222	0.555370	-1.529336
O	0.702945	1.795536	0.931800
C	1.756742	2.719562	0.646789
H	2.065209	2.556507	-0.397799
H	1.333482	3.724021	0.781383
H	2.609747	2.578206	1.327418
23			
TS-C1C2 SCF Done: -1298.96291155 A.U.			
C	1.521217	-0.134342	-0.250681
C	1.955435	1.123914	0.214051
C	3.264643	1.246923	0.675236
C	4.108086	0.131786	0.665246
C	3.585188	-1.072715	0.185197
N	2.335498	-1.209049	-0.258970
H	3.623113	2.212530	1.042152
H	1.276066	1.972831	0.203878
H	5.140095	0.189428	1.017725
H	4.211128	-1.973170	0.159849
C	0.153599	-0.376164	-0.731078
C	-1.039921	0.519944	-0.762633
O	-2.155038	0.088349	-1.064054
K	-3.041879	-0.966806	1.168137
H	-0.441336	1.013666	1.746296
N	-0.159399	-1.624353	-0.972623
N	-0.492968	-2.693776	-1.160588
O	-1.220941	0.534449	1.440238

O	-0.697530	1.817701	-0.878666
C	-1.749292	2.751365	-0.640529
H	-2.090261	2.628753	0.399261
H	-1.320727	3.751308	-0.793385
H	-2.589940	2.595960	-1.334124
23			
C2 SCF Done: -1298.97161220 A.U.			
C	1.563364	-0.183753	-0.170238
C	2.058667	1.057342	0.292178
C	3.392037	1.143013	0.685894
C	4.209693	0.011027	0.603228
C	3.634739	-1.168405	0.118049
N	2.359119	-1.274341	-0.252702
H	3.792813	2.093915	1.048033
H	1.402357	1.926439	0.308172
H	5.260697	0.038041	0.898658
H	4.243036	-2.077364	0.028445
C	0.167139	-0.358119	-0.568643
C	-1.067740	0.582586	-0.332234
O	-2.161927	0.162385	-0.842798
K	-3.238505	-1.055567	1.048822
H	-0.403339	0.973170	1.568607
N	-0.190118	-1.541790	-0.968592
N	-0.597066	-2.549319	-1.314497
O	-1.225904	0.648574	1.171807
O	-0.617677	1.882279	-0.734708
C	-1.631319	2.864676	-0.727583
H	-2.035486	3.030078	0.288838
H	-1.178794	3.803045	-1.084419
H	-2.468651	2.590499	-1.391738
23			
TS-C2C3 SCF Done: -1298.96449305 A.U.			
C	1.543338	0.134517	-0.144925
C	1.465099	-1.262874	0.029813
C	2.650816	-1.996695	0.028554
C	3.869579	-1.326261	-0.110956
C	3.841440	0.068018	-0.225947
N	2.716594	0.785209	-0.253533
H	2.623480	-3.081675	0.161728
H	0.485728	-1.709696	0.237069
H	4.820892	-1.862728	-0.113065
H	4.779276	0.630980	-0.305925
C	0.319716	0.951351	-0.197451
C	-1.048589	0.547094	-0.632598
O	-2.002943	1.314498	-0.543398
K	-3.598865	-0.857628	-0.250038
H	-0.383901	-1.071250	-1.467981
N	0.415808	2.203746	0.169295
N	0.483886	3.289892	0.489333
O	-1.107977	-0.435829	-1.588855
O	-1.374694	-0.912984	0.924958
C	-1.058701	-0.388834	2.153588
H	0.022244	-0.497189	2.429455
H	-1.271641	0.709222	2.234243
H	-1.622948	-0.858047	2.997409

23

C3 SCF Done: -1298.96763972 A.U.

C	-1.604137	0.167786	-0.309461
C	-2.414659	1.155171	0.283638
C	-3.742929	0.839337	0.566033
C	-4.232650	-0.431741	0.253962
C	-3.351962	-1.339071	-0.341694
N	-2.079029	-1.054098	-0.616554
H	-4.391435	1.588138	1.028431
H	-2.013557	2.138372	0.517131
H	-5.266540	-0.714792	0.462063
H	-3.692630	-2.346729	-0.607735
C	-0.185864	0.379745	-0.657620
C	0.749140	1.456482	-0.341674
O	1.899387	1.511210	-0.758196
K	3.738807	-0.271206	0.089311
H	0.929142	3.073400	0.591931
N	0.405509	-0.634340	-1.265987
N	0.916961	-1.497140	-1.775454
O	0.232711	2.406850	0.445361
O	1.853116	-0.986427	1.247780
C	0.744540	-1.407078	1.892766
H	0.069817	-0.581312	2.271190
H	0.044124	-2.045626	1.276085
H	0.929075	-2.036342	2.814696

23

TS-C3C' SCF Done: -1298.96458711 A.U.

C	1.525826	0.195183	-0.149795
C	1.468082	-1.211355	-0.141769
C	2.666236	-1.921451	-0.218491
C	3.873851	-1.219550	-0.257585
C	3.824693	0.177578	-0.202425
N	2.686238	0.872998	-0.161993
H	2.655561	-3.014689	-0.218977
H	0.497614	-1.702769	0.002313
H	4.834081	-1.737269	-0.310587
H	4.752822	0.761352	-0.197991
C	0.290300	1.011993	-0.123817
C	-1.004231	0.770890	-0.775042
O	-1.949621	1.538646	-0.676393
K	-3.589710	-0.685309	-0.243854
H	-0.561850	-1.004414	-1.309979
N	0.354854	2.157914	0.519062
N	0.408708	3.142383	1.072371
O	-1.074743	-0.252729	-1.656856
O	-1.436958	-1.258108	0.805369
C	-0.976380	-1.180693	2.087644
H	-0.103844	-1.855526	2.313085
H	-0.605631	-0.157822	2.381261
H	-1.732536	-1.439102	2.878755

23

C' SCF Done: -1299.02339209 A.U.

C	2.120929	0.041170	-0.010219
C	2.145392	-1.366331	-0.112459
C	3.380025	-2.011368	-0.115586
C	4.554451	-1.257113	-0.018557

C	4.426678	0.131637	0.078583
N	3.254651	0.767704	0.083522
H	3.424340	-3.101302	-0.193995
H	1.203485	-1.906741	-0.185918
H	5.540543	-1.726684	-0.017966
H	5.321603	0.761650	0.156341
C	0.864156	0.804464	0.000713
C	-0.567753	0.330146	-0.080497
O	-1.452689	1.224249	-0.039565
K	-3.971069	1.030345	-0.087021
H	-2.330931	-1.295209	-0.164502
N	0.987922	2.109792	0.099022
N	1.063959	3.236535	0.182168
O	-0.758415	-0.908963	-0.183683
O	-3.323310	-1.454280	-0.098241
C	-3.543496	-2.767452	0.359361
H	-3.052179	-2.965314	1.333277
H	-4.626672	-2.927699	0.494701
H	-3.182568	-3.532424	-0.357648

23

TS-CD' SCF Done: -1299.00459273 A.U.

C	-1.987335	0.017163	-0.021796
C	-2.060282	1.426910	-0.154313
C	-3.311998	2.023598	-0.162763
C	-4.476986	1.239386	-0.042092
C	-4.329625	-0.136765	0.084290
N	-3.118367	-0.701586	0.091389
H	-3.393599	3.109135	-0.264109
H	-1.131175	1.987055	-0.244651
H	-5.471665	1.689084	-0.046599
H	-5.188976	-0.807686	0.182025
C	-0.778773	-0.792073	0.008252
C	0.649406	-0.393236	-0.083438
O	1.515895	-1.305259	-0.020927
K	4.024981	-1.151351	-0.114207
H	2.429956	1.187473	-0.202507
N	-1.154311	-2.073365	0.146011
N	-2.224466	-2.551234	0.233183
O	0.882152	0.843885	-0.221868
O	3.428631	1.347609	-0.123809
C	3.633780	2.611607	0.457113
H	4.712881	2.764232	0.632375
H	3.286042	3.440632	-0.193130
H	3.119360	2.719605	1.433775

23

D' SCF Done: -1299.03601187 A.U.

C	1.875984	0.116432	-0.040156
C	2.112554	1.506135	-0.179093
C	3.413611	1.956147	-0.170554
C	4.498824	1.038147	-0.024625
C	4.260283	-0.303544	0.108466
N	2.959102	-0.732522	0.097663
H	3.626786	3.022305	-0.275615
H	1.247702	2.159549	-0.287014
H	5.529858	1.395436	-0.017908
H	5.020909	-1.076563	0.224154

C	0.772742	-0.756934	0.006170
C	-0.679075	-0.396285	-0.092620
O	-1.529405	-1.316570	-0.023577
K	-4.046216	-1.206213	-0.100948
H	-2.477070	1.161842	-0.221915
N	1.248627	-2.014154	0.162012
N	2.551789	-2.021611	0.218793
O	-0.918593	0.837016	-0.243277
O	-3.476709	1.303786	-0.135112
C	-3.698570	2.555709	0.466454
H	-3.369910	3.399850	-0.174071
H	-4.778689	2.687243	0.651822
H	-3.178581	2.657686	1.440745

23

A_pyridazine SCF Done: -534.304425411 A.U.

N	2.939091	-1.236214	-0.064479
C	3.454250	-0.376966	0.811685
C	2.911714	0.897182	1.039328
C	1.789507	1.242997	0.308540
C	1.287417	0.295844	-0.605490
N	1.863502	-0.900790	-0.769739
H	3.363799	1.577151	1.765048
H	4.340147	-0.722571	1.353924
H	1.298487	2.211912	0.426020
C	0.037718	0.558980	-1.414566
H	0.010368	1.616317	-1.716586
H	0.091579	-0.055896	-2.325969
C	-1.222421	0.214450	-0.637382
C	-2.126720	1.210709	-0.242077
C	-1.487202	-1.118761	-0.279863
C	-3.275791	0.884125	0.488278
H	-1.932416	2.252982	-0.511642
C	-2.633080	-1.446974	0.448515
H	-0.779370	-1.899133	-0.572955
C	-3.532583	-0.445451	0.835432
H	-3.971918	1.673177	0.785971
H	-2.825921	-2.489560	0.716165
H	-4.429752	-0.702169	1.405145

26

B_pyridazine SCF Done: -725.820290138 A.U.

C	1.353127	0.114878	0.320567
C	1.701829	-0.916548	1.216345
C	3.738410	-1.075302	-0.008030
N	2.186873	0.485201	-0.659542
H	1.007926	-1.209938	2.006723
H	4.720756	-1.517335	-0.200032
C	0.011223	0.817453	0.428198
H	-0.117871	1.150398	1.472730
Li	1.454964	2.025753	-1.676864
N	-0.004099	1.982904	-0.473103
N	-0.909604	2.887356	-0.239589
O	-1.697960	2.711000	0.712030
C	-1.118169	-0.166312	0.119008
C	-1.110815	-0.888302	-1.085432
C	-2.185599	-0.346908	1.009699
C	-2.146219	-1.776755	-1.391177

H	-0.284849	-0.757346	-1.790568
C	-3.219131	-1.239284	0.709246
H	-2.210232	0.233297	1.934432
C	-3.204013	-1.956475	-0.492767
H	-2.125553	-2.332857	-2.332579
H	-4.045319	-1.369434	1.413860
H	-4.014505	-2.651317	-0.729067
N	3.371879	-0.103466	-0.830980
C	2.929616	-1.524682	1.052558
H	3.271532	-2.325259	1.712053
26			
TS-BC_pyridazine SCF Done: -725.782060766 A.U.			
C	1.301014	-0.100995	0.091096
C	1.608650	-1.214091	0.925979
C	3.802686	-1.154520	-0.018554
N	2.263311	0.395021	-0.732768
H	0.856958	-1.601255	1.615374
H	4.826397	-1.529874	-0.108336
C	0.017281	0.589613	0.131222
H	-0.266180	1.517647	1.276537
Li	1.590223	1.838213	-1.883953
N	0.067993	1.848424	-0.649930
N	-0.232311	2.875298	0.026450
O	-0.552594	2.638793	1.277174
C	-1.267978	-0.156226	0.003220
C	-1.332405	-1.552652	-0.211642
C	-2.502866	0.536649	0.056215
C	-2.554606	-2.219712	-0.330022
H	-0.415052	-2.134801	-0.311793
C	-3.721276	-0.131260	-0.075606
H	-2.513658	1.616087	0.213586
C	-3.762209	-1.517910	-0.261029
H	-2.557723	-3.301138	-0.495889
H	-4.651659	0.442195	-0.027451
H	-4.717519	-2.039969	-0.358992
N	3.493602	-0.117342	-0.776739
C	2.873667	-1.747593	0.867001
H	3.168629	-2.591504	1.495063
23			
D_pyridazine SCF Done: -642.494443199 A.U.			
N	-3.457671	0.561976	0.059023
C	-3.816004	-0.686787	-0.111495
C	-2.903558	-1.775361	-0.268845
C	-1.553687	-1.528355	-0.225198
C	-1.137446	-0.190311	-0.018016
N	-2.138787	0.769511	0.090547
H	-3.293463	-2.781981	-0.426021
H	-4.895541	-0.861161	-0.135561
H	-0.816446	-2.321257	-0.352506
C	0.042138	0.570088	0.085086
C	1.454270	0.164152	0.041889
C	2.434022	1.099611	-0.346494
C	1.864537	-1.135626	0.395325
C	3.781132	0.739223	-0.392528
H	2.125026	2.111433	-0.616065
C	3.214142	-1.493680	0.342266

H	1.132172	-1.866603	0.743159
C	4.177475	-0.560203	-0.053879
H	4.527315	1.476899	-0.699615
H	3.514897	-2.506571	0.622930
H	5.232970	-0.841716	-0.093785
N	-0.327859	1.867838	0.226227
N	-1.628403	1.997025	0.234030
23			
A_pyrimidine_i SCF Done: -534.341685407 A.U.			
C	-1.290589	0.028141	-0.676940
N	-1.746961	1.207238	-0.232176
C	-2.794327	1.182444	0.596487
C	-3.398473	-0.011318	0.994378
C	-2.846734	-1.183306	0.475270
N	-1.799470	-1.168992	-0.354405
H	-3.166554	2.148729	0.956910
H	-4.254079	-0.027084	1.671860
H	-3.261617	-2.164271	0.735655
C	-0.061400	0.047299	-1.560698
H	-0.081426	0.960865	-2.171539
H	-0.093716	-0.827977	-2.224804
C	1.201179	0.014398	-0.717687
C	1.818958	1.206102	-0.307182
C	1.733753	-1.208840	-0.279541
C	2.952103	1.176375	0.512229
H	1.403908	2.164629	-0.630821
C	2.866218	-1.240641	0.540032
H	1.250122	-2.142267	-0.580732
C	3.480091	-0.047467	0.937800
H	3.424929	2.113500	0.819058
H	3.271663	-2.201515	0.868980
H	4.367118	-0.071453	1.576617
26			
B_pyrimidine_i SCF Done: -725.853652012 A.U.			
C	1.360390	0.065568	0.277426
C	2.709195	-1.711765	0.776054
C	3.658810	-1.287004	-0.158269
C	3.360560	-0.119473	-0.850350
N	2.220234	0.557434	-0.635622
H	2.872918	-2.618324	1.370064
H	4.584639	-1.837022	-0.332764
H	4.048678	0.291566	-1.595968
C	0.043999	0.793917	0.523800
H	-0.038898	0.959073	1.612661
Li	1.529646	2.295034	-1.340379
N	0.062211	2.076924	-0.184083
N	-0.862532	2.933880	0.147780
O	-1.692551	2.598410	1.015292
C	-1.119912	-0.119584	0.128082
C	-1.727713	-0.952626	1.078523
C	-1.557707	-0.181381	-1.202762
C	-2.756307	-1.823626	0.709336
H	-1.392013	-0.913638	2.117947
C	-2.588207	-1.051075	-1.575010
H	-1.097531	0.469989	-1.949931
C	-3.191001	-1.877049	-0.620500

H	-3.224360	-2.461683	1.464326
H	-2.922618	-1.082134	-2.615912
H	-3.997887	-2.556023	-0.909514
N	1.575214	-1.045324	0.989055
26			
TS-BC_pyrimidine_i SCF Done: -725.818881202 A.U.			
C	1.340959	-0.127177	0.029393
C	2.710752	-1.921692	0.485989
C	3.820776	-1.277780	-0.072768
C	3.575819	-0.016913	-0.607719
N	2.366917	0.554052	-0.573851
H	2.806940	-2.929656	0.908468
H	4.809337	-1.737154	-0.100513
H	4.375798	0.553817	-1.092825
C	0.050782	0.550896	0.136859
H	-0.292060	1.241318	1.350371
Li	1.714758	2.175383	-1.504046
N	0.115664	1.896682	-0.453226
N	-0.274064	2.808140	0.347861
O	-0.672277	2.378126	1.507902
C	-1.258410	-0.156806	-0.037000
C	-1.450723	-1.522902	0.273305
C	-2.390698	0.564236	-0.483031
C	-2.700172	-2.130278	0.126625
H	-0.603561	-2.102010	0.635518
C	-3.639260	-0.047031	-0.620729
H	-2.297355	1.620784	-0.738990
C	-3.808233	-1.401911	-0.319615
H	-2.806967	-3.190891	0.374018
H	-4.488238	0.547279	-0.971552
H	-4.785510	-1.880112	-0.426674
N	1.506627	-1.366073	0.542536
23			
D_pyrimidine_i SCF Done: -642.520453862 A.U.			
C	-1.146055	0.163265	0.000101
N	-1.427016	1.479348	-0.000131
C	-2.696712	1.823933	-0.000215
C	-3.769954	0.879194	-0.000188
C	-3.475780	-0.457062	-0.000075
N	-2.153909	-0.799680	0.000108
H	-2.924772	2.895162	-0.000159
H	-4.806947	1.215741	-0.000194
H	-4.197145	-1.276175	0.000058
C	0.035136	-0.605876	-0.000086
C	1.440694	-0.183003	-0.000068
C	1.793654	1.180997	0.000250
C	2.467123	-1.148797	-0.000324
C	3.136981	1.563921	0.000308
H	1.008753	1.938953	0.000518
C	3.806861	-0.759302	-0.000295
H	2.201745	-2.207619	-0.000553
C	4.149473	0.598406	0.000027
H	3.393615	2.626773	0.000598
H	4.590610	-1.521770	-0.000495
H	5.199868	0.901320	0.000063
N	-1.638706	-2.042616	0.000503

N	-0.339548	-1.909401	0.000028
23			
A_pyrimidine_o SCF Done: -534.342206627 A.U.			
C	3.604009	-0.383082	0.016468
N	3.652443	0.951924	0.016587
C	2.471917	1.579285	0.000650
C	1.258471	0.890457	-0.014805
C	1.319106	-0.508877	-0.013645
N	2.507344	-1.137349	0.002440
H	2.488526	2.675627	0.000548
H	4.565156	-0.911695	0.029614
H	0.307027	1.422728	-0.027016
C	0.096364	-1.405691	-0.032469
H	0.182117	-2.044254	-0.927902
H	0.185833	-2.087433	0.829796
C	-1.237045	-0.697848	-0.013796
C	-1.869927	-0.327780	-1.211265
C	-1.852010	-0.359700	1.202587
C	-3.086923	0.361257	-1.195256
H	-1.402216	-0.583073	-2.166776
C	-3.068801	0.329173	1.222920
H	-1.370011	-0.640017	2.143889
C	-3.690241	0.692321	0.022921
H	-3.567127	0.638328	-2.137779
H	-3.534909	0.581257	2.179431
H	-4.642422	1.229409	0.037156
26			
B_pyrimidine_o SCF Done: -725.855739268 A.U.			
C	1.351169	0.115572	0.316018
C	1.701663	-0.912778	1.201708
C	2.939538	-1.519315	1.024807
C	3.375249	-0.177131	-0.750102
N	2.206162	0.477281	-0.661514
H	3.269241	-2.324265	1.691003
H	1.021107	-1.222674	1.996440
H	4.048590	0.134443	-1.556412
C	0.009444	0.817224	0.426223
H	-0.118283	1.146446	1.472174
Li	1.444367	2.028245	-1.676398
N	-0.004578	1.984222	-0.470815
N	-0.904320	2.893366	-0.232419
O	-1.690965	2.718251	0.720463
C	-1.121928	-0.164082	0.116320
C	-1.121046	-0.879146	-1.092229
C	-2.185473	-0.347902	1.010836
C	-2.158611	-1.765072	-1.397780
H	-0.298332	-0.745610	-1.800716
C	-3.221558	-1.237206	0.710102
H	-2.205006	0.226905	1.939054
C	-3.212597	-1.948182	-0.495591
H	-2.142726	-2.316536	-2.341987
H	-4.044744	-1.369986	1.417710
H	-4.024940	-2.640833	-0.731900
N	3.781967	-1.156372	0.044496
26			

TS-BC_pyrimidine_o SCF Done: -725.820188016 A.U.

C	1.291666	-0.109261	0.082552
C	1.579072	-1.250713	0.878296
C	2.855611	-1.775251	0.832648
C	3.502768	-0.193906	-0.649134
N	2.301828	0.398270	-0.691692
H	3.116681	-2.647046	1.443579
H	0.820683	-1.678895	1.534185
H	4.279465	0.251938	-1.283227
C	0.017556	0.583504	0.103638
H	-0.215932	1.495612	1.239203
Li	1.609284	1.824935	-1.885280
N	0.072926	1.838093	-0.684651
N	-0.191156	2.870642	0.000557
O	-0.483158	2.640652	1.255224
C	-1.281825	-0.148450	-0.000257
C	-1.363899	-1.531512	-0.277023
C	-2.504467	0.553213	0.126276
C	-2.595792	-2.181847	-0.388153
H	-0.453832	-2.113637	-0.429379
C	-3.733664	-0.096888	0.001840
H	-2.496980	1.623939	0.335391
C	-3.792722	-1.472405	-0.248027
H	-2.615886	-3.254277	-0.603245
H	-4.656639	0.480587	0.107541
H	-4.755819	-1.981183	-0.339816
N	3.840665	-1.255000	0.066340

23

D_pyrimidine_o SCF Done: -642.520499384 A.U.

C	3.470293	-0.463245	0.030418
N	3.869150	0.762320	-0.091928
C	2.931002	1.758565	-0.193054
C	1.575910	1.529208	-0.159538
C	1.138226	0.187993	-0.012439
N	2.134771	-0.776315	0.065986
H	3.320538	2.773734	-0.306723
H	4.159756	-1.309252	0.108497
H	0.863063	2.347882	-0.249650
C	-0.046452	-0.569570	0.061639
C	-1.458032	-0.162854	0.029630
C	-2.453210	-1.122028	-0.248564
C	-1.855997	1.163734	0.283181
C	-3.800197	-0.760428	-0.281078
H	-2.156940	-2.154629	-0.441887
C	-3.205822	1.522365	0.244801
H	-1.113072	1.921386	0.535592
C	-4.184076	0.564071	-0.038841
H	-4.556922	-1.518459	-0.500313
H	-3.493869	2.557476	0.446643
H	-5.239815	0.845962	-0.067269
N	1.611236	-2.017095	0.171850
N	0.320184	-1.876190	0.165261

23

A_pyrazine SCF Done: -534.331243180 A.U.

C	-3.595090	0.402361	0.169086
C	-3.542947	-0.993280	0.078383

N	-2.384377	-1.631648	-0.098012
C	-1.283572	-0.880605	-0.183358
C	-1.325100	0.522881	-0.096020
N	-2.495922	1.151768	0.082735
H	-4.551621	0.916674	0.317104
H	-4.455796	-1.594760	0.151242
H	-0.331030	-1.399570	-0.325286
C	-0.094932	1.402697	-0.218154
H	-0.153247	1.914686	-1.194337
H	-0.187434	2.193674	0.543598
C	1.232008	0.691531	-0.085780
C	1.952368	0.287051	-1.220415
C	1.753968	0.390068	1.183204
C	3.164111	-0.400808	-1.092697
H	1.558203	0.513266	-2.215579
C	2.964011	-0.297073	1.315066
H	1.203142	0.697775	2.077070
C	3.673486	-0.695563	0.176091
H	3.712593	-0.705917	-1.988123
H	3.356515	-0.520593	2.310921
H	4.620901	-1.231624	0.277887

26

B_pyrazine SCF Done: -725.844310822 A.U.

C	1.357839	0.132015	0.302935
C	1.722287	-0.888772	1.203385
C	3.711751	-1.175853	0.133634
C	3.375230	-0.169071	-0.768132
N	2.203933	0.481740	-0.679757
H	1.032328	-1.174621	2.004541
H	4.669685	-1.699556	0.053396
H	4.057230	0.120812	-1.572785
C	0.010525	0.821219	0.420023
H	-0.118564	1.155913	1.463989
Li	1.423202	2.025532	-1.703134
N	-0.012734	1.984764	-0.483004
N	-0.917840	2.889833	-0.249018
O	-1.701709	2.716747	0.706234
C	-1.116302	-0.167131	0.115434
C	-1.106322	-0.898701	-1.083244
C	-2.185492	-0.341770	1.005331
C	-2.140229	-1.790664	-1.383950
H	-0.279331	-0.773386	-1.788218
C	-3.217535	-1.237452	0.709970
H	-2.211798	0.245033	1.925801
C	-3.199543	-1.964250	-0.486213
H	-2.117096	-2.354608	-2.320631
H	-4.044522	-1.363255	1.414432
H	-4.008606	-2.662188	-0.718216
N	2.882569	-1.530929	1.123520

26

TS-BC_pyrazine SCF Done: -725.806194053 A.U.

C	1.309833	-0.075903	0.075471
C	1.631030	-1.183721	0.916704
C	3.761019	-1.272570	0.096209
C	3.490333	-0.186290	-0.724368
N	2.283595	0.403800	-0.746092

H	0.876714	-1.564232	1.612845
H	4.747564	-1.745625	0.102112
H	4.259678	0.222070	-1.387999
C	0.018384	0.599814	0.123738
H	-0.276335	1.512624	1.272828
Li	1.547252	1.845355	-1.902865
N	0.059796	1.862663	-0.647164
N	-0.251467	2.883445	0.034943
O	-0.577190	2.634198	1.280138
C	-1.262314	-0.155180	-0.002222
C	-1.316947	-1.554382	-0.200482
C	-2.501565	0.530615	0.037056
C	-2.534291	-2.230194	-0.317162
H	-0.395633	-2.132337	-0.286647
C	-3.715279	-0.146517	-0.092313
H	-2.520517	1.611659	0.181464
C	-3.746686	-1.535257	-0.262031
H	-2.529670	-3.313580	-0.469375
H	-4.649355	0.421696	-0.054736
H	-4.698236	-2.064540	-0.357779
N	2.816711	-1.764175	0.922766

23

D_pyrazine SCF Done: -642.512933471 A.U.

C	-3.471920	0.474893	-0.034468
C	-3.789239	-0.849549	0.101476
N	-2.853770	-1.841502	0.210713
C	-1.583228	-1.517686	0.168387
C	-1.147818	-0.172737	0.011763
N	-2.139542	0.793632	-0.070382
H	-4.183253	1.297390	-0.111870
H	-4.839726	-1.149567	0.133866
H	-0.843386	-2.317415	0.265832
C	0.044106	0.581232	-0.063618
C	1.453924	0.167342	-0.030716
C	1.846527	-1.158916	-0.292886
C	2.451151	1.121299	0.256968
C	3.194791	-1.522956	-0.254116
H	1.100940	-1.911635	-0.552673
C	3.796562	0.754418	0.290063
H	2.157457	2.153234	0.457515
C	4.175408	-0.569896	0.038804
H	3.479642	-2.557514	-0.462765
H	4.555854	1.507567	0.516826
H	5.230025	-0.855927	0.067536
N	-0.315587	1.882152	-0.171331
N	-1.616694	2.021318	-0.178171

22

A_triazine SCF Done: -550.373466455 A.U.

C	-1.296034	-0.023806	0.667308
N	-1.771457	-1.195825	0.222609
C	-2.805347	-1.116804	-0.613264
C	-2.833675	1.127961	-0.525422
N	-1.801398	1.167068	0.315572
H	-3.218605	-2.058568	-0.993965
H	-3.270484	2.086191	-0.831577
C	-0.081521	-0.044203	1.562284

H	-0.110280	-0.958092	2.171750
H	-0.118039	0.833615	2.222417
C	1.184722	-0.015537	0.721988
C	1.790551	-1.210418	0.303682
C	1.729978	1.206889	0.298660
C	2.927873	-1.184090	-0.509748
H	1.364587	-2.167549	0.616847
C	2.866817	1.234364	-0.514953
H	1.255332	2.142418	0.607194
C	3.469886	0.038560	-0.920828
H	3.392796	-2.122859	-0.823152
H	3.283822	2.193926	-0.832730
H	4.360098	0.059498	-1.555207
N	-3.378392	0.016459	-1.023869

25

B triazine SCF Done: -741.883654170 A.U.

C	-1.358332	0.040191	-0.274202
C	-2.699937	-1.729608	-0.710974
C	-3.350121	-0.209949	0.809762
N	-2.240961	0.518669	0.625002
H	-2.893761	-2.652796	-1.269306
H	-4.076138	0.160739	1.541891
C	-0.061393	0.790080	-0.520726
H	0.012889	0.958334	-1.610404
Li	-1.584996	2.281103	1.343832
N	-0.107972	2.067237	0.193783
N	0.795497	2.946990	-0.139914
O	1.626723	2.633325	-1.012846
C	1.116336	-0.110281	-0.131895
C	1.722838	-0.941593	-1.084370
C	1.567066	-0.156714	1.194920
C	2.767167	-1.795735	-0.720503
H	1.375639	-0.913798	-2.120330
C	2.613557	-1.009769	1.560893
H	1.106438	0.493980	1.942203
C	3.216752	-1.833504	0.604840
H	3.235707	-2.432372	-1.476223
H	2.959951	-1.029386	2.598020
H	4.036181	-2.499162	0.889271
N	-1.564917	-1.087432	-0.963065
N	-3.627260	-1.338915	0.171289

25

TS-BC triazine SCF Done: -741.854562703 A.U.

C	1.329561	-0.156393	0.011796
C	2.692941	-1.943542	0.397132
C	3.565836	-0.106894	-0.542879
N	2.391952	0.520771	-0.538597
H	2.816124	-2.969672	0.765421
H	4.415306	0.435159	-0.976411
C	0.063641	0.539009	0.118902
H	-0.206727	1.189505	1.326001
Li	1.790642	2.178525	-1.466810
N	0.152678	1.888727	-0.465545
N	-0.189721	2.797359	0.362869
O	-0.555909	2.367705	1.525405
C	-1.265611	-0.144736	-0.040252

C	-1.496297	-1.485909	0.336184
C	-2.365891	0.588777	-0.535083
C	-2.761007	-2.064276	0.200583
H	-0.671496	-2.072404	0.735797
C	-3.629823	0.006970	-0.662416
H	-2.234691	1.629136	-0.836965
C	-3.839453	-1.326312	-0.298458
H	-2.903165	-3.107433	0.498126
H	-4.457090	0.606333	-1.053484
H	-4.828335	-1.781737	-0.397605
N	1.481362	-1.422784	0.466428
N	3.789734	-1.333539	-0.078976
22			
D triazine SCF Done: -658.546819460 A.U.			
C	-3.469004	-0.389954	-0.000164
N	-3.765639	0.873590	-0.000160
C	-2.733860	1.777885	-0.000218
C	-1.146342	0.175675	0.000053
N	-2.160653	-0.780562	-0.000030
H	-3.021034	2.833512	0.000008
H	-4.223919	-1.183422	-0.000165
C	0.027273	-0.594323	0.000129
C	1.435337	-0.181567	0.000098
C	2.454458	-1.154108	-0.000229
C	1.793706	1.180638	0.000306
C	3.796293	-0.771570	-0.000291
H	2.183426	-2.211463	-0.000417
C	3.138787	1.556191	0.000171
H	1.014182	1.944366	0.000445
C	4.145295	0.584271	-0.000110
H	4.576111	-1.537876	-0.000560
H	3.401565	2.617380	0.000276
H	5.197267	0.881467	-0.000175
N	-1.655013	-2.029032	0.000250
N	-0.359671	-1.899958	0.000230
N	-1.456060	1.486993	0.000012
22			
A triazine_3 SCF Done: -550.297840696 A.U.			
C	1.290076	0.296881	0.600027
C	2.959055	0.828524	-0.977015
N	1.823379	-0.936145	0.680731
H	3.483790	1.488703	-1.674513
C	0.054776	0.559089	1.423647
H	0.037340	1.615626	1.727107
H	0.113611	-0.061991	2.330213
C	-1.208950	0.222330	0.646679
C	-2.069110	1.234154	0.196352
C	-1.515739	-1.114507	0.341889
C	-3.218944	0.918373	-0.536852
H	-1.840687	2.278958	0.425490
C	-2.662458	-1.430971	-0.390768
H	-0.842897	-1.907974	0.678226
C	-3.518802	-0.414778	-0.832374
H	-3.882074	1.718507	-0.876986
H	-2.889603	-2.476136	-0.617890
H	-4.416801	-0.662813	-1.404517

N	3.447703	-0.415041	-0.862390
C	1.852761	1.248484	-0.253122
H	1.445859	2.257776	-0.343654
N	2.873984	-1.268263	-0.040378
25			
B_triazine_3 SCF Done: -741.811189968 A.U.			
C	-1.346496	0.080570	-0.329555
C	-2.921015	-1.557482	-0.964873
N	-2.214737	0.457499	0.626393
H	-3.293284	-2.384635	-1.575931
C	-0.024127	0.810617	-0.432608
H	0.096977	1.141453	-1.479408
Li	-1.523264	2.038222	1.649313
N	-0.046139	1.976236	0.465403
N	0.844458	2.897850	0.236752
O	1.644271	2.730295	-0.705259
C	1.121624	-0.153409	-0.121436
C	2.176957	-0.337930	-1.025102
C	1.137650	-0.852535	1.096099
C	3.224128	-1.213433	-0.723168
H	2.182158	0.224939	-1.960885
C	2.186621	-1.724734	1.402162
H	0.321266	-0.715786	1.811449
C	3.233020	-1.909021	0.491551
H	4.042001	-1.347171	-1.436604
H	2.185651	-2.263967	2.353412
H	4.054272	-2.590777	0.728531
N	-3.743167	-1.136406	0.016462
C	-1.683822	-0.978594	-1.179684
H	-1.004485	-1.321218	-1.962335
N	-3.382725	-0.150060	0.788645
25			
TS-BC_triazine_3 SCF Done: -741.778805275 A.U.			
C	-1.272852	-0.150474	-0.097467
C	-2.812369	-1.810376	-0.817981
N	-2.311780	0.357872	0.640239
H	-3.110359	-2.693083	-1.391274
C	-0.027848	0.575301	-0.089594
H	0.149686	1.509214	-1.188587
Li	-1.732639	1.798233	1.874097
N	-0.118563	1.803566	0.743016
N	0.102835	2.861716	0.081275
O	0.376228	2.679491	-1.181933
C	1.289279	-0.133363	-0.004079
C	1.395609	-1.489036	0.372661
C	2.491801	0.569054	-0.244483
C	2.638560	-2.120585	0.471621
H	0.498570	-2.062546	0.614140
C	3.733202	-0.059637	-0.129773
H	2.456426	1.620816	-0.533290
C	3.817429	-1.411826	0.220346
H	2.683109	-3.173214	0.765408
H	4.644189	0.513710	-0.323441
H	4.789699	-1.904281	0.304140
N	-3.795651	-1.239354	-0.073081
C	-1.532352	-1.316514	-0.863138

H	-0.760175	-1.776281	-1.481041
N	-3.517671	-0.180975	0.631185
22			
D triazine_3 SCF Done: -658.478057925 A.U.			
N	3.867405	0.648595	0.000021
C	2.988662	1.702451	0.000102
C	1.143475	0.217318	-0.000008
N	2.137019	-0.760927	-0.000075
H	3.455769	2.688650	0.000172
C	-0.044213	-0.538626	-0.000050
C	-1.460230	-0.142046	-0.000013
C	-2.455473	-1.140839	0.000285
C	-1.863001	1.206714	-0.000271
C	-3.807246	-0.797653	0.000328
H	-2.155994	-2.190037	0.000488
C	-3.218103	1.545750	-0.000222
H	-1.123665	2.007206	-0.000529
C	-4.196633	0.546947	0.000079
H	-4.563528	-1.587075	0.000564
H	-3.508800	2.599448	-0.000428
H	-5.256523	0.814040	0.000117
N	1.619648	-1.992059	-0.000094
N	0.324513	-1.847728	-0.000138
C	1.623357	1.543761	0.000091
H	0.953590	2.402896	0.000143
N	3.470784	-0.561850	-0.000063
22			
A triazine_2_1 SCF Done: -550.324805173 A.U.			
C	1.306568	-0.137297	0.622085
C	2.648079	1.311921	-0.486174
N	2.005993	-1.204711	0.221719
H	2.920340	2.333306	-0.775934
C	0.083965	-0.388032	1.471858
H	0.106064	0.312231	2.320858
H	0.139634	-1.413753	1.860268
C	-1.193946	-0.191582	0.675063
C	-1.778497	1.079509	0.559698
C	-1.782656	-1.271564	-0.001475
C	-2.932841	1.265096	-0.207507
H	-1.321379	1.929175	1.073474
C	-2.937651	-1.087875	-0.768444
H	-1.329882	-2.264354	0.074054
C	-3.516732	0.181505	-0.873327
H	-3.379425	2.260337	-0.284047
H	-3.387421	-1.940232	-1.285020
H	-4.420884	0.325851	-1.470852
N	3.063950	-1.027016	-0.562388
C	3.396645	0.205806	-0.925232
H	4.271520	0.317293	-1.572533
N	1.593460	1.136759	0.292164
25			
B triazine_2_1 SCF Done: -741.837622593 A.U.			
C	-1.357950	0.041565	-0.284309
C	-2.689236	-1.731305	-0.747785
N	-2.224274	0.523715	0.617258

H	-2.895552	-2.649466	-1.309375
C	-0.059721	0.793056	-0.521441
H	0.019527	0.970389	-1.609101
Li	-1.594299	2.271969	1.350042
N	-0.106773	2.066204	0.203236
N	0.804608	2.942608	-0.117334
O	1.640523	2.630610	-0.986649
C	1.114376	-0.111349	-0.133143
C	1.740681	-0.918431	-1.093483
C	1.540807	-0.189100	1.200468
C	2.780811	-1.778592	-0.731179
H	1.413332	-0.865632	-2.135054
C	2.582846	-1.047892	1.565129
H	1.063165	0.440630	1.955116
C	3.206293	-1.846803	0.600778
H	3.265096	-2.395634	-1.493227
H	2.909893	-1.091882	2.607793
H	4.022411	-2.516912	0.884313
N	-1.563791	-1.086014	-0.988561
C	-3.602936	-1.246442	0.210781
H	-4.537161	-1.767472	0.437323
N	-3.358028	-0.128377	0.872599
25			
TS-BC_triazine_2_1 SCF Done: -741.805345458 A.U.			
C	1.332393	-0.161458	0.022206
C	2.698248	-1.942409	0.432648
N	2.367105	0.519662	-0.561342
H	2.842005	-2.962088	0.810101
C	0.062232	0.535716	0.134765
H	-0.235762	1.216731	1.342293
Li	1.793566	2.173604	-1.473518
N	0.152068	1.880941	-0.460910
N	-0.204703	2.797257	0.350935
O	-0.585957	2.377194	1.516168
C	-1.261246	-0.151582	-0.034279
C	-1.487036	-1.499157	0.325747
C	-2.367567	0.580265	-0.521032
C	-2.748779	-2.082417	0.184549
H	-0.661173	-2.087627	0.720356
C	-3.628533	-0.006492	-0.653349
H	-2.243167	1.624327	-0.812695
C	-3.832152	-1.344848	-0.304485
H	-2.884847	-3.129750	0.470351
H	-4.458888	0.593409	-1.037195
H	-4.818886	-1.804003	-0.407588
N	3.578937	-0.007384	-0.612442
N	1.491740	-1.423605	0.499163
C	3.778948	-1.216835	-0.110561
H	4.792591	-1.622154	-0.159492
22			
D_triazine_2_1 SCF Done: -658.510141362 A.U.			
C	2.729761	1.787314	0.000028
C	1.145596	0.184079	0.000001
N	2.158831	-0.776397	-0.000029
H	3.024205	2.841030	0.000049
C	-0.028504	-0.588067	-0.000016

C	-1.437129	-0.176159	-0.000001
C	-2.454161	-1.150890	0.000184
C	-1.797722	1.185336	-0.000167
C	-3.796570	-0.770886	0.000199
H	-2.180383	-2.207504	0.000318
C	-3.143418	1.558534	-0.000149
H	-1.019830	1.950757	-0.000306
C	-4.147845	0.584471	0.000034
H	-4.575125	-1.538439	0.000345
H	-3.408394	2.619157	-0.000280
H	-5.200377	0.879690	0.000048
N	1.662814	-2.012317	-0.000051
N	0.358422	-1.889104	-0.000026
N	3.463598	-0.510615	-0.000036
N	1.452449	1.493625	0.000031
C	3.743810	0.767335	-0.000010
H	4.804189	1.032579	-0.000016

22

A_triazine_2 SCF Done: -550.325268219 A.U.

C	1.295747	0.279443	0.600704
C	0.056052	0.565815	1.408758
H	0.042887	1.628378	1.692640
H	0.109158	-0.034453	2.329835
C	-1.209285	0.221224	0.638590
C	-2.087014	1.224508	0.203607
C	-1.502971	-1.117446	0.328586
C	-3.240563	0.898696	-0.519572
H	-1.868793	2.270813	0.436185
C	-2.653649	-1.444362	-0.392963
H	-0.816736	-1.904624	0.653353
C	-3.527282	-0.436278	-0.819499
H	-3.916659	1.692552	-0.848717
H	-2.870450	-2.490979	-0.623620
H	-4.428119	-0.692131	-1.383694
N	2.932786	-1.221926	0.002643
C	1.834635	1.211478	-0.313545
H	1.380695	2.202190	-0.434062
C	3.402752	-0.314629	-0.847184
H	4.281213	-0.606272	-1.432093
N	1.866367	-0.918658	0.736373
N	2.897457	0.912559	-1.041119

25

B_triazine_2 SCF Done: -741.838290100 A.U.

C	-1.353135	0.103638	-0.310087
N	-2.221284	0.478317	0.629993
C	-0.026454	0.821043	-0.424202
H	0.093926	1.154064	-1.470547
Li	-1.520821	2.059154	1.651063
N	-0.037213	1.985378	0.476621
N	0.863963	2.897996	0.253468
O	1.662902	2.726362	-0.688259
C	1.112423	-0.153137	-0.118658
C	2.171927	-0.332999	-1.018686
C	1.117512	-0.867998	1.089922
C	3.211879	-1.218606	-0.722004
H	2.185291	0.241229	-1.947399

C	2.159764	-1.750053	1.391162
H	0.297889	-0.735468	1.802272
C	3.209969	-1.929294	0.484122
H	4.032582	-1.348943	-1.432810
H	2.150146	-2.301293	2.335467
H	4.025527	-2.619348	0.716718
C	-3.656763	-1.151094	-0.063909
H	-4.622292	-1.648451	0.070429
N	-3.388823	-0.154224	0.764456
N	-2.849555	-1.595199	-1.044592
C	-1.693544	-0.973592	-1.164269
H	-0.994904	-1.303471	-1.941213
25			
TS-BC_triazine_2 SCF Done: -741.803335996 A.U.			
C	-1.289282	-0.114625	-0.078243
N	-2.299762	0.355456	0.695942
C	-0.029918	0.597280	-0.099903
H	0.186889	1.550799	-1.207949
Li	-1.684456	1.798546	1.905928
N	-0.104600	1.827091	0.729263
N	0.145564	2.882856	0.076545
O	0.434788	2.698048	-1.186064
C	1.270386	-0.134727	-0.000963
C	1.347035	-1.502340	0.341989
C	2.491813	0.549024	-0.203958
C	2.575676	-2.161758	0.438621
H	0.437102	-2.064493	0.561701
C	3.718256	-0.107456	-0.089162
H	2.482420	1.608341	-0.465880
C	3.771906	-1.470807	0.223418
H	2.594560	-3.222701	0.704014
H	4.642950	0.453019	-0.253788
H	4.733094	-1.984558	0.306916
N	-3.505305	-0.218459	0.664778
C	-3.692355	-1.260886	-0.117760
H	-4.691164	-1.706980	-0.117183
C	-1.567061	-1.255451	-0.901194
H	-0.785560	-1.662875	-1.551929
N	-2.750749	-1.815529	-0.921135
22			
D_triazine_2 SCF Done: -658.514037357 A.U.			
C	-1.153175	-0.205098	-0.000014
N	-2.141095	0.775165	-0.000107
C	0.040808	0.546134	-0.000144
C	1.455629	0.144733	-0.000052
C	2.452796	1.141771	0.000408
C	1.854707	-1.204960	-0.000422
C	3.803686	0.795724	0.000498
H	2.154924	2.191326	0.000704
C	3.208821	-1.547007	-0.000323
H	1.113422	-2.004032	-0.000821
C	4.189315	-0.549986	0.000137
H	4.562030	1.583082	0.000863
H	3.497327	-2.601232	-0.000625
H	5.248581	-0.819627	0.000210
N	-1.623791	1.995243	-0.000627

N	-0.321148	1.852509	-0.000297
N	-3.458179	0.552434	-0.000017
C	-3.782362	-0.715824	0.000234
H	-4.854736	-0.929887	0.000294
C	-1.642822	-1.536149	0.000270
H	-0.953567	-2.385429	0.000415
N	-2.931844	-1.782528	0.000393
22			
A_triazine_1 SCF Done: -550.326414155 A.U.			
C	1.289916	-0.224502	0.622872
C	2.785596	1.240517	-0.241751
H	3.161444	2.265774	-0.327097
C	0.060748	-0.522306	1.443846
H	0.098649	0.105108	2.347490
H	0.071694	-1.576877	1.753338
C	-1.207638	-0.223052	0.659657
C	-1.613702	1.105172	0.449521
C	-1.967989	-1.260700	0.100588
C	-2.761242	1.387510	-0.296246
H	-1.018587	1.919898	0.869958
C	-3.117775	-0.979238	-0.645830
H	-1.659595	-2.298918	0.253817
C	-3.517763	0.345606	-0.846087
H	-3.067632	2.426129	-0.447923
H	-3.702592	-1.799262	-1.071379
H	-4.416593	0.566843	-1.427820
N	3.025273	-0.945409	-0.857444
N	1.721065	1.031517	0.541197
C	1.973278	-1.226698	-0.100604
H	1.657614	-2.273692	-0.060462
N	3.444380	0.315483	-0.935997
25			
B_triazine_1 SCF Done: -741.836710513 A.U.			
C	-1.350715	0.105051	-0.297060
N	-2.242839	0.483974	0.619811
C	-0.027556	0.824021	-0.420827
H	0.088247	1.143652	-1.472440
Li	-1.528554	2.094753	1.622338
N	-0.039985	1.997013	0.464824
N	0.857353	2.910389	0.228238
O	1.654588	2.728495	-0.712491
C	1.113501	-0.146327	-0.110937
C	2.155766	-0.352120	-1.025215
C	1.136221	-0.831873	1.114177
C	3.197189	-1.234857	-0.725539
H	2.155120	0.198967	-1.968015
C	2.179678	-1.711693	1.417575
H	0.330409	-0.678091	1.837997
C	3.212999	-1.917028	0.496817
H	4.004966	-1.385369	-1.447027
H	2.184245	-2.240779	2.374468
H	4.029569	-2.605120	0.731530
N	-2.824217	-1.632527	-1.029727
C	-1.673235	-0.991725	-1.131272
H	-0.971141	-1.341436	-1.893602
C	-3.388697	-0.222461	0.676465

H	-4.127239	0.071488	1.428342
N	-3.704044	-1.244772	-0.100781
25			
TS-BC_triazine_1 SCF Done: -741.806426952 A.U.			
C	-1.280494	-0.121346	-0.061760
N	-2.337855	0.358737	0.646689
C	-0.033420	0.593795	-0.063146
H	0.122777	1.512793	-1.158687
Li	-1.721219	1.791139	1.899535
N	-0.114144	1.820193	0.771709
N	0.094305	2.878687	0.105516
O	0.348281	2.696756	-1.158855
C	1.282336	-0.121414	0.008040
C	1.386390	-1.460216	0.439657
C	2.480850	0.559557	-0.299695
C	2.626010	-2.100319	0.525074
H	0.490619	-2.012194	0.732224
C	3.719658	-0.076111	-0.196579
H	2.443409	1.598626	-0.631418
C	3.801708	-1.413313	0.207738
H	2.671065	-3.140374	0.860171
H	4.629501	0.478557	-0.442525
H	4.771813	-1.911548	0.282034
C	-1.518485	-1.300711	-0.843847
H	-0.715272	-1.741195	-1.441166
N	-2.691120	-1.881994	-0.908991
N	-3.730613	-1.374363	-0.207867
C	-3.502198	-0.298577	0.523053
H	-4.354639	0.090969	1.090996
22			
D_triazine_1 SCF Done: -658.497513769 A.U.			
C	-1.158275	-0.163184	-0.000035
N	-2.167270	0.799346	0.000028
C	0.027716	0.605773	0.000007
C	1.432620	0.184353	0.000006
C	2.455092	1.153952	0.000127
C	1.784744	-1.179343	-0.000117
C	3.794959	0.766388	0.000127
H	2.187475	2.212123	0.000223
C	3.128349	-1.559757	-0.000116
H	1.001802	-1.939433	-0.000210
C	4.137993	-0.591256	0.000007
H	4.578024	1.529271	0.000223
H	3.387278	-2.621798	-0.000211
H	5.188814	-0.892488	0.000008
N	-1.659234	2.032223	0.000052
N	-0.351509	1.902376	0.000043
C	-3.687515	-0.941424	-0.000017
H	-4.702047	-1.342941	-0.000018
N	-2.677972	-1.865655	-0.000075
N	-1.439416	-1.478809	-0.000083
C	-3.471528	0.414177	0.000037
H	-4.238475	1.190820	0.000074