

Supplementary Information

Computational Assessments on Diastereoselective [4+2] Cycloaddition and 1,3-Borotopic Shift of Dearomatized Tertiary Boronic Ester Intermediate: Reactivities Explained Through Transition-State Distortion Energies

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Supplementary data:

Cartesian coordinates, electronic energies and free energies of all stationary points during the reaction pathways. All provided geometries were optimized at the specified level of theory. All energies are either in gas phase or tetrahydrofuran (THF) or chloroform (CHCl_3) at 298.15 K in Hartree.

8				N	-2.3925105	-0.6940893	-0.3123915
C	0.7085895	2.7640837	-0.6000405	C	-3.8712595	-0.6448963	-0.4029805
C	0.1346025	1.6322867	-0.0047455	O	-4.4055685	-1.1835673	0.6748665
C	-1.2724185	1.6183547	0.0613285	C	-5.8410325	-1.1228233	0.7443925
C	-2.0527175	2.6695417	-0.4361755	H	-6.2779065	-1.6356533	-0.1138995
C	-1.4481135	3.7700827	-1.0260865	H	-6.1015305	-1.6241763	1.6739535
C	-0.0563725	3.8116717	-1.1033165	H	-6.1667375	-0.0811173	0.7581065
H	1.7925195	2.8001157	-0.6630015	C	-1.9023625	-2.0074243	0.2352365
H	-3.1386545	2.6209767	-0.3608145	H	-2.2732075	-2.1286243	1.2508095
H	-2.0503515	4.5877017	-1.4112495	H	-2.2739105	-2.8123383	-0.4025245
H	0.4318355	4.6712957	-1.5559355	H	-0.8079095	-1.9499993	0.2073535
B	1.1020755	0.4169157	0.5598995	C	-1.8063305	-0.5032483	-1.6796745
C	0.8335125	0.0758857	2.1505695	H	-2.1452835	0.4434287	-2.0899345
C	0.2393285	1.0630747	3.1440675	H	-0.7245615	-0.5179423	-1.5398245
C	1.6977555	0.7201417	3.2050625	H	-2.1441115	-1.3331803	-2.3026935
H	0.5907975	-0.9691513	2.3689165	O	-4.4457585	-0.1461913	-1.3251965
H	-0.4018095	0.6980857	3.9450045	$E_{\text{gas}} = -1161.90821533$			
H	-0.0387545	2.0469397	2.7708295	$E_{\text{THF}} = -1161.93952173$			
H	2.0455395	0.1227927	4.0447975	$G_{\text{gas}} = -1161.4543273$			
H	2.4159185	1.4559387	2.8537865	$G_{\text{THF}} = -1161.485634$			
O	2.4990635	0.7641977	0.2616205				
C	3.1605855	-0.3823593	-0.2117425	9			
C	2.0341385	-1.1187033	-1.0156355	C	0.4302659	2.3386161	-1.4111607
O	0.8757955	-0.8576453	-0.2396235	C	0.1615929	1.4034571	-0.3688957
C	3.6684125	-1.2243463	0.9712605	C	-1.1769971	1.4465081	0.2248513
H	4.2936795	-2.0616853	0.6393375	C	-2.1550371	2.4007581	-0.2723737
H	2.8385195	-1.6162043	1.5649145	C	-1.8441231	3.2384581	-1.2872907
H	4.2672275	-0.5796673	1.6217225	C	-0.5338431	3.1880461	-1.8706807
C	4.3554015	0.0559597	-1.0568525	H	1.4111439	2.3054151	-1.8748607
H	5.1006435	0.5347107	-0.4133425	H	-3.1448981	2.3996571	0.1723673
H	4.8314075	-0.7991103	-1.5522325	H	-2.5760581	3.9394791	-1.6741967
H	4.0526145	0.7820047	-1.8154005	H	-0.3198951	3.8316111	-2.7206627
C	2.2176605	-2.6300293	-1.1343295	B	1.3636439	0.5599361	0.2049953
H	1.3971715	-3.0618493	-1.7203665	C	1.4848909	1.7560521	1.4425443
H	3.1580405	-2.8769633	-1.6409575	C	1.7294749	3.2444421	1.3639383
H	2.2167235	-3.1041773	-0.1497845	C	2.8551809	2.3327001	1.7240163
C	1.8535435	-0.5171873	-2.4179845	H	0.8741029	1.4396701	2.2906173
H	2.7140025	-0.7180653	-3.0654315	H	1.2949029	3.8713391	2.1378613
H	0.9734935	-0.9617273	-2.8978885	H	1.7466799	3.7080251	0.3792473
H	1.7043475	0.5647477	-2.3544825	H	3.2112259	2.3115801	2.7515233
C	-1.9634995	0.4585647	0.6963225	H	3.6151789	2.1485901	0.9721263
H	-1.3124595	-0.0333163	1.4158745	O	2.5248389	0.4745581	-0.6439887
H	-2.8898135	0.7479607	1.1965055	C	3.1392289	-0.7843609	-0.4051377

C	1.9251349	-1.6688359	0.0348103
O	1.1288619	-0.7505619	0.7787333
C	4.1818349	-0.6461749	0.7119993
H	4.7356549	-1.5793439	0.8625943
H	3.7093089	-0.3611979	1.6560883
H	4.8973919	0.1344471	0.4359463
C	3.8316579	-1.2371669	-1.6874167
H	4.6644609	-0.5623479	-1.9099727
H	4.2343469	-2.2514199	-1.5824387
H	3.1465739	-1.2143479	-2.5379857
C	2.2776199	-2.8502539	0.9308603
H	1.3696889	-3.4108719	1.1781193
H	2.9720689	-3.5321799	0.4269933
H	2.7305959	-2.5131849	1.8659123
C	1.1214519	-2.1590449	-1.1768407
H	1.6724349	-2.9102109	-1.7526877
H	0.1888849	-2.6143019	-0.8329227
H	0.8740429	-1.3257969	-1.8427287
C	-1.5134731	0.6057571	1.2356913
H	-0.8047391	-0.1244339	1.6134163
H	-2.5010441	0.6440191	1.6878163
N	-3.1127181	-1.3085189	-0.6417427
C	-4.1410141	-0.5748559	-0.1442127
O	-4.5659031	-1.0471019	1.0536953
C	-5.6864211	-0.3586919	1.5962693
H	-6.5435031	-0.4161949	0.9209783
H	-5.9082391	-0.8617729	2.5376083
H	-5.4505191	0.6938371	1.7749293
C	-2.5077641	-2.4299189	0.0522873
H	-1.5361341	-2.1463349	0.4760963
H	-3.1626541	-2.7770449	0.8484043
H	-2.3478111	-3.2473919	-0.6600007
C	-2.4597501	-0.8719269	-1.8587127
H	-1.4142511	-0.6122379	-1.6543757
H	-2.4808451	-1.6736889	-2.6062697
H	-2.9790951	0.0030161	-2.2466857
O	-4.6376351	0.4017421	-0.6790977

$E_{\text{gas}} = -1161.88752863$

$E_{\text{THF}} = -1161.90784125$

$G_{\text{gas}} = -1161.4428396$

$G_{\text{THF}} = -1161.463152$

Imaginary frequency = -121.3927

N(Me)₂CO₂Me

N	0.8343591	-0.0506971	-0.0892616
C	-0.4463519	-0.5159971	-0.0348856
O	-0.7628829	-1.6903401	-0.0142006
O	-1.3468329	0.4934689	-0.0214016
C	-2.7051889	0.0710389	-0.0010976
H	-2.9131339	-0.5269901	0.8895364
H	-3.2940409	0.9887509	0.0113544
H	-2.9422459	-0.5212731	-0.8884616

C	1.1884661	1.3506869	-0.0014246
H	1.5565331	1.6050809	1.0022154
H	1.9833741	1.5690719	-0.7236696
H	0.3258481	1.9723939	-0.2304226
C	1.9206941	-1.0023101	0.0080034
H	2.6554961	-0.8144231	-0.7835916
H	2.4280591	-0.9204111	0.9788824
H	1.5178471	-2.0080501	-0.1015756

$E_{\text{gas}} = -363.059514899$

$E_{\text{THF}} = -363.067371224$

$G_{\text{gas}} = -362.954054$

$G_{\text{THF}} = -362.961910$

10a

C	-2.1999184	-0.6427890	-1.4054879
C	-1.6775154	0.1637680	-0.2356589
C	-2.1890344	-0.3528350	1.1241961
C	-3.2242154	-1.3866910	1.1308391
C	-3.6583804	-1.9788000	0.0067481
C	-3.1158324	-1.6095950	-1.2963449
H	-1.8106594	-0.3627860	-2.3815049
H	-3.6337264	-1.6696880	2.0977631
H	-4.4244674	-2.7474860	0.0552021
H	-3.4720404	-2.1335520	-2.1786199
C	-1.7249814	0.1428640	2.2832271
H	-0.9545724	0.9054760	2.3176691
H	-2.1239934	-0.2019520	3.2336151
B	-0.1000344	-0.0131840	-0.1808969
O	0.7771856	0.8834180	0.3766181
O	0.5217646	-1.1368670	-0.6521429
C	1.9439306	-0.9159620	-0.5638229
C	2.0414186	0.2015240	0.5300401
C	2.4030396	-0.4463820	-1.9454579
H	3.4887716	-0.3153510	-1.9872219
H	1.9261886	0.5005450	-2.2181999
H	2.1142056	-1.1967250	-2.6865649
C	2.6247326	-2.2272370	-0.1993169
H	3.6971556	-2.0717950	-0.0381019
H	2.5019956	-2.9462090	-1.0144929
H	2.1928256	-2.6637600	0.7035151
C	3.1661996	1.2057990	0.3273271
H	3.1402056	1.9537590	1.1250161
H	3.0718376	1.7258700	-0.6281649
H	4.1395676	0.7043630	0.3607941
C	2.0712376	-0.3521280	1.9552971
H	3.0221276	-0.8486770	2.1717551
H	1.2553396	-1.0628030	2.1207551
H	1.9445016	0.4749410	2.6599051
C	-2.1704854	1.6021830	-0.4580279
C	-1.4678014	2.5621250	-1.3815379
H	-3.2578164	1.6455940	-0.4952339
H	-2.0686004	3.1717220	-2.0496059

H -0.5073284 2.2627770 -1.7942889
C -1.5129994 2.8325680 0.1014591
H -2.1654774 3.6226530 0.4606831
H -0.5843504 2.7213040 0.6482681
E_{gas} = -798.884925121
E_{THF} = -798.901886562
E_{CHCl3} = -798.903975979
G_{gas} = -798.563204
G_{THF} = -798.580166
G_{CHCl3} = -798.561710

10b

C 0.1331926 1.8882826 -1.5197685
C 0.1554126 1.2427436 -0.1433295
C 0.2903956 2.2995886 0.9617525
C 0.8483286 3.6068046 0.6017995
C 0.9509406 4.0165446 -0.6721045
C 0.5096286 3.1507726 -1.7572445
H -0.2049544 1.2651446 -2.3426105
H 1.1381996 4.2650266 1.4177265
H 1.3357526 5.0049876 -0.9058715
H 0.4815816 3.5492586 -2.7678845
C -0.0459044 2.0826426 2.2431345
H -0.5339294 1.1750296 2.5763245
H 0.1302756 2.8467196 2.9964775
B -1.2403124 0.4785736 -0.0573445
O -2.2574414 0.7775926 0.8068915
O -1.5749344 -0.5369624 -0.9229465
C -2.9850894 -0.7943024 -0.7730765
C -3.2705194 -0.2368864 0.6634735
C -3.2327234 -2.2861924 -0.9434445
H -4.2834104 -2.5262764 -0.7471425
H -2.6057804 -2.8757474 -0.2711345
H -3.0013884 -2.5830014 -1.9706665
C -3.6942404 -0.0104844 -1.8787745
H -4.7732924 -0.1932284 -1.8742235
H -3.2926664 -0.3255624 -2.8461555
H -3.5198514 1.0649716 -1.7737615
C -3.0277084 -1.2657884 1.7695855
H -3.0522254 -0.7562624 2.7370675
H -2.0476264 -1.7412014 1.6627055
H -3.7955204 -2.0454174 1.7681665
C -4.6385484 0.4067406 0.8395995
H -5.4331344 -0.3262624 0.6614465
H -4.7761214 1.2473756 0.1566435
H -4.7411314 0.7813316 1.8621375
C 1.1683126 -0.7896954 1.1002485
H 1.0919106 -0.2361864 2.0427185
H 0.2273616 -1.3413124 0.9624905
C 2.3290266 -1.7927864 1.1908705
H 2.1530476 -2.4673714 2.0379855

C 1.3691116 0.1938656 -0.0712885
C 2.7150766 0.9229556 0.1385735
H 2.6814836 1.5020436 1.0679815
H 2.8778986 1.6341986 -0.6812815
C 3.6472446 -1.0328814 1.4002125
H 4.4810746 -1.7425664 1.4840395
H 3.6079166 -0.4656584 2.3395315
C 3.8786726 -0.0795434 0.2177245
H 4.8149486 0.4717596 0.3681955
C 3.9608196 -0.8934954 -1.0809145
H 4.1494206 -0.2257854 -1.9318965
H 4.7979586 -1.6028294 -1.0323395
C 2.4008536 -2.6030524 -0.1109615
H 1.4636436 -3.1554624 -0.2609785
H 3.2096066 -3.3437394 -0.0544145
C 1.4868046 -0.6315224 -1.3755345
H 0.5447406 -1.1496724 -1.5801685
H 1.6801346 0.0417726 -2.2187785
C 2.6382706 -1.6450474 -1.2863195
H 2.6794066 -2.2145454 -2.2231425
E_{gas} = -1071.72287714
E_{THF} = -1071.74122845
G_{gas} = -1071.243481
G_{THF} = -1071.261779

11a

N -3.6922273 0.6172429 -0.0000913
N -3.6922243 -0.6172511 -0.0000913
C -2.2917633 1.1187709 0.0000067
C -2.2917573 -1.1187721 0.0000167
O -2.0298413 2.2836369 -0.0000983
O -2.0298293 -2.2836361 -0.0000873
N -1.4656953 0.0000009 -0.0000443
C -0.0272553 0.0000019 -0.0000423
C 0.6683427 -1.2110621 -0.0000153
C 0.6683447 1.2110649 -0.0000073
C 2.0588397 -1.1988451 0.0000517
H 0.1380797 -2.1523281 -0.0000293
C 2.0588417 1.1988459 0.0000597
H 0.1380837 2.1523319 -0.0000153
C 2.7622307 -0.0000001 0.0000797
H 2.5901177 -2.1453651 0.0000817
H 2.5901217 2.1453649 0.0000957
H 3.8475917 -0.0000011 0.0001297
E_{gas} = -622.491779919
E_{THF} = -622.508053488
G_{gas} = -622.399144
G_{THF} = -622.415417

11b

C -1.0794867 0.4145247 0.7247103

C	0.0922933	0.1434067	0.6241283
C	1.4897133	-0.2520633	0.5432953
C	-2.4798967	0.7946787	0.8966623
O	1.9179983	-1.2787463	1.0087683
O	-3.3613507	0.2307797	0.0630923
O	-2.8222467	1.5755057	1.7434073
O	2.2052823	0.6634237	-0.1103857
C	3.5992323	0.3610087	-0.2403987
H	3.7353293	-0.5705323	-0.7943797
H	4.0265023	1.2001857	-0.7867947
H	4.0601783	0.2664747	0.7452123
C	-2.9136157	-0.7085773	-0.9147917
H	-2.2041547	-0.2479303	-1.6081707
H	-2.4552157	-1.5810703	-0.4407577
H	-3.8105627	-1.0110683	-1.4535977

$E_{\text{gas}} = -533.058678752$

$E_{\text{THF}} = -533.073401014$

$G_{\text{gas}} = -532.980743$

$G_{\text{THF}} = -532.995465$

11c

C	1.0105279	0.2187243	0.0074694
H	2.0670949	0.4487553	0.0149964
C	-0.0409121	1.0331063	0.0089424
H	-0.0823891	2.1136173	0.0180064
C	0.5044019	-1.1849777	-0.0075946
C	-1.2734751	0.1920583	-0.0051046
O	-0.8764561	-1.1315567	-0.0146316
O	-2.4194581	0.5222473	-0.0085706
O	1.1106659	-2.2119747	-0.0135136

$E_{\text{gas}} = -379.283986181$

$E_{\text{THF}} = -379.298773160$

$G_{\text{gas}} = -379.256155$

$G_{\text{THF}} = -379.270942$

11d

C	1.1403347	-1.5046945	-0.5617262
C	-2.3753383	-0.0113715	-0.0847792
O	1.6363667	-2.5047215	-1.0247972
O	-2.9191703	1.1598445	0.2997768
O	-3.1029183	-0.9042755	-0.4396362
O	1.8469717	-0.5066695	-0.0075252
C	-0.3241493	-1.2540415	-0.5477812
H	-0.9331823	-2.0411645	-0.9803402
C	-0.8861293	-0.1522775	-0.0490822
H	-0.2631893	0.6237665	0.3797458
C	3.2613297	-0.7001625	0.0088688
H	3.6480537	-0.7851855	-1.0094952
H	3.6714917	0.1804105	0.5020888

H	3.5165867	-1.6057405	0.5641558
C	-2.1159993	2.2735645	0.6644738
H	-1.5473823	2.0793615	1.5800448
H	-1.4371193	2.5654915	-0.1435302
H	-2.8165573	3.0878655	0.8495378

$E_{\text{gas}} = -534.328924015$

$E_{\text{THF}} = -534.345069352$

$G_{\text{gas}} = -534.225893$

$G_{\text{THF}} = -534.242038$

11e

C	-0.3667179	0.4788656	-0.8297616
C	1.9562761	-0.4522854	0.8640244
O	-0.1974889	-0.7157184	-0.9492076
O	2.9977691	-0.5011844	0.2646064
C	0.2564951	1.3230066	0.2158314
H	-0.1002249	2.3435056	0.3074504
C	1.2378211	0.8676176	0.9947214
H	1.6785871	1.5327976	1.7341004
C	0.2071451	-1.4775534	2.1313064
H	0.1099941	-2.4199994	2.6699204
H	-0.5650059	-1.4073274	1.3626454
H	0.1161891	-0.6462604	2.8380724
C	-1.7957879	0.4743146	-2.6794056
H	-2.3701369	1.2102936	-3.2405316
H	-2.4545769	-0.2912734	-2.2623046
H	-1.0524229	-0.0059084	-3.3196406
O	-1.1554629	1.2041226	-1.6312866
O	1.4975491	-1.5170134	1.5294584

$E_{\text{gas}} = -534.326627208$

$E_{\text{THF}} = -534.343213397$

$G_{\text{gas}} = -534.222878$

$G_{\text{THF}} = -534.239464$

11f

C	-0.9875867	0.2023288	0.4099495
C	-0.6874407	0.3516118	-0.9457495
C	-0.0240277	-0.2197622	1.3223305
C	0.5975103	0.0720548	-1.3838935
H	-1.4675037	0.6827728	-1.6227695
C	1.2635683	-0.4987392	0.8765425
H	-0.3032887	-0.3214892	2.3665995
C	1.5702373	-0.3521302	-0.4740515
H	0.8501083	0.1821338	-2.4339715
H	2.0249133	-0.8285792	1.5760155
H	2.5749383	-0.5693962	-0.8243355
N	-2.2906607	0.4662538	0.9686045
O	-3.1207677	0.8329408	0.1647295

$E_{\text{gas}} = -361.516638404$

$E_{\text{THF}} = -361.526012271$

$G_{\text{gas}} = -361.448223$

G_{THF} = -361.457597

12a-syn

C	0.0715324	-1.3525160	-1.2770529
C	-1.1309076	-1.6168590	-0.4044939
C	-0.7543266	-2.4239890	0.8332361
C	0.6731654	-2.7371910	1.0218701
C	1.5233114	-2.8372970	-0.0832729
C	1.2239724	-2.0907360	-1.2372149
H	-0.0797206	-0.6401770	-2.0829209
H	0.9419834	-3.2583460	1.9347951
H	2.4812474	-3.3350830	0.0215641
H	1.9743484	-1.9738540	-2.0136809
C	-1.6452526	-2.8676610	1.7235891
H	-2.7050766	-2.6660460	1.6156831
H	-1.3346006	-3.4395450	2.5932621
B	-1.7129236	-0.1836040	-0.0066499
O	-2.4044746	0.0874050	1.1370771
O	-1.6970176	0.8559270	-0.8962509
C	-2.5167586	1.9111990	-0.3549459
C	-2.6309726	1.5150320	1.1644541
C	-3.8508586	1.8556380	-1.1007019
H	-4.5273126	2.6529130	-0.7773429
H	-4.3505846	0.8926240	-0.9541799
H	-3.6626756	1.9777080	-2.1715149
C	-1.8180026	3.2387960	-0.6152939
H	-2.3486186	4.0620050	-0.1242419
H	-1.7990346	3.4372810	-1.6909649
H	-0.7849596	3.2125010	-0.2633919
C	-3.9944296	1.7736720	1.7904751
H	-3.9829146	1.4518820	2.8359011
H	-4.7875976	1.2270560	1.2752651
H	-4.2310456	2.8430240	1.7649871
C	-1.5308226	2.1233180	2.0344711
H	-1.6724426	3.2016450	2.1573311
H	-0.5439496	1.9366830	1.6053441
H	-1.5635376	1.6515960	3.0205751
N	0.8202974	-0.0266000	0.7162751
N	1.3039454	-0.9152390	1.5244121
C	1.8873754	0.6368880	0.0455121
C	2.7597244	-0.9407350	1.4148921
O	1.7769424	1.5913310	-0.6806089
O	3.4909714	-1.6346800	2.0715191
N	3.0788504	0.0334830	0.4838661
C	4.3928784	0.3759170	0.0625301
C	5.3513124	-0.6270550	-0.0786389
C	4.7121424	1.7055320	-0.2094569
C	6.6369224	-0.2918050	-0.4873699
H	5.0977854	-1.6556600	0.1476361
C	5.9984434	2.0234240	-0.6309369
H	3.9572404	2.4746450	-0.1087769

C	6.9644634	1.0313540	-0.7685749
H	7.3840194	-1.0729300	-0.5887509
H	6.2440354	3.0585830	-0.8470309
H	7.9686714	1.2874910	-1.0920269
C	-2.1326186	-2.4135850	-1.2619489
C	-2.9493866	-1.7637090	-2.3473189
H	-1.7857266	-3.4235800	-1.4717629
H	-3.1040246	-2.3214270	-3.2656739
H	-2.8510686	-0.6912860	-2.4821809
C	-3.6213326	-2.2568270	-1.0927599
H	-4.2353436	-3.1502910	-1.1502799
H	-3.9752616	-1.5182390	-0.3783119

E_{gas} = -1421.38288820

E_{THF} = -1421.41299828

G_{gas} = -1420.944557

G_{THF} = -1420.974667

Imaginary frequency = -379.0411

12a-anti

C	-0.3175722	0.0249612	0.7323906
C	0.6850408	-0.9858998	0.2225116
C	0.2569598	-1.5607148	-1.1291494
C	-0.8173482	-0.8685508	-1.8285984
C	-1.2782822	0.3675652	-1.4508024
C	-1.0014942	0.8501142	-0.1548644
H	-0.1693942	0.3615602	1.7525586
H	-1.1772512	-1.3169958	-2.7503184
H	-1.9775852	0.9017672	-2.0868134
H	-1.4634412	1.7635132	0.2033416
C	0.8396148	-2.6279958	-1.6890684
H	1.6502688	-3.1580858	-1.2029114
H	0.5142008	-2.9962178	-2.6574744
B	2.0264269	-0.1363108	0.0168016
O	3.0051038	-0.4561108	-0.8770714
O	2.3091118	0.9811902	0.7549426
C	3.4583218	1.6092872	0.1418406
C	4.1351088	0.4036662	-0.5953984
C	4.3055388	2.2565162	1.2266936
H	5.2246689	2.6702712	0.7977906
H	4.5737838	1.5415732	2.0072226
H	3.7483348	3.0747592	1.6917436
C	2.9133219	2.6711852	-0.8145424
H	3.7209938	3.2404262	-1.2845454
H	2.2825868	3.3632132	-0.2497114
H	2.2995879	2.2193782	-1.6003904
C	5.0846589	-0.3916138	0.3011146
H	5.3461779	-1.3266408	-0.2025564
H	4.6150598	-0.6403328	1.2581876
H	6.0064758	0.1636572	0.4995806
C	4.8177318	0.7568652	-1.9080844
H	5.6210228	1.4824292	-1.7397594
H	4.1098779	1.1761322	-2.6260644
H	5.2560868	-0.1426178	-2.3495394

N -1.9286392 -1.1525288 1.0822326
N -2.1976981 -1.9153678 0.0801456
C -3.0205362 -0.2040788 1.3034266
C -3.4673812 -1.5414338 -0.4655764
O -3.0810402 0.5829212 2.2109986
O -4.0321512 -2.0903108 -1.3751334
N -3.9527222 -0.4802058 0.3186896
C -5.1941412 0.1877072 0.1397776
C -6.3128541 -0.5294838 -0.2824814
C -5.2813861 1.5575422 0.3862046
C -7.5198512 0.1357902 -0.4641794
H -6.2303612 -1.5903758 -0.4812574
C -6.4985601 2.2064212 0.2127706
H -4.4105012 2.1027322 0.7296176
C -7.6194701 1.5014862 -0.2156894
H -8.3888601 -0.4228458 -0.7978944
H -6.5673062 3.2715622 0.4114446
H -8.5667502 2.0133922 -0.3540614
C 0.9054368 -2.0946528 1.2547336
C 1.6956969 -1.8494288 2.5115716
H 0.0308358 -2.7303868 1.3580916
H 1.3234829 -2.2791588 3.4358096
H 2.1774908 -0.8824518 2.6331286
C 2.2322008 -2.7772048 1.4510666
H 2.2208529 -3.8446808 1.6483936
H 3.0805139 -2.4469038 0.8591116

$E_{\text{gas}} = -1421.38206737$

$E_{\text{THF}} = -1421.41574754$

$G_{\text{gas}} = -1420.945165$

$G_{\text{THF}} = -1420.978846$

Imaginary frequency = -302.7626

12b-syn

C 0.5616402 -0.8182934 -0.4329633
C -0.5587548 -0.4367094 0.5125697
C -0.1535478 -0.7660684 1.9484307
C 1.0876692 -1.5438264 2.1286487
C 1.6357062 -2.3059874 1.0914837
C 1.4013672 -1.8873274 -0.2235583
H 0.5505162 -0.3417824 -1.4074533
H 1.3634692 -1.7841994 3.1502037
H 2.3899892 -3.0527264 1.3141777
H 2.0187312 -2.2665644 -1.0332253
C -0.7832368 -0.3437394 3.0509117
H -1.6378288 0.3192636 3.0167797
H -0.4142998 -0.6184914 4.0353277
B -0.7423548 1.1363156 0.3141657
O -1.1234528 2.0279216 1.2752597
O -0.5915808 1.7078356 -0.9207823
C -1.0197608 3.0802446 -0.8244493
C -0.9365698 3.3499556 0.7199117
C -2.4463108 3.1343796 -1.3741643

H -2.8326398 4.1581146 -1.3968693
H -3.1259628 2.5184036 -0.7761113
H -2.4454778 2.7418786 -2.3953493
C -0.0897288 3.9369006 -1.6717263
H -0.2972928 5.0016966 -1.5186693
H -0.2403728 3.7088206 -2.7310453
H 0.9558812 3.7362866 -1.4301313
C -2.0210818 4.2669866 1.2666377
H -1.8827918 4.3973956 2.3438287
H -3.0192498 3.8560656 1.0994067
H -1.9621478 5.2534026 0.7939407
C 0.4427682 3.8290396 1.1733527
H 0.6381352 4.8525696 0.8385277
H 1.2289892 3.1695486 0.7971367
H 0.4808362 3.8056026 2.2661967
N 1.9639842 0.6629136 0.7766497
N 2.3267892 0.0169516 1.8460497
C 3.0271972 0.6316246 -0.1749453
C 3.6537142 -0.5454404 1.6538157
O 3.0528702 1.2253536 -1.2220653
O 4.2689912 -1.1677014 2.4808887
N 4.0548662 -0.1411274 0.3899877
C 5.2981372 -0.4424284 -0.2285753
C 6.4570002 -0.5207614 0.5426577
C 5.3449982 -0.6626774 -1.6049373
C 7.6654402 -0.8258304 -0.0736063
H 6.4065142 -0.3602224 1.6122677
C 6.5628452 -0.9539644 -2.2083043
H 4.4407602 -0.5847904 -2.1961453
C 7.7252142 -1.0394794 -1.4474293
H 8.5669152 -0.8902794 0.5279397
H 6.5995882 -1.1172664 -3.2810153
H 8.6732752 -1.2697294 -1.9235143
C -4.3276278 -2.8002384 0.6929167
H -5.2501708 -3.3199674 0.4028847
H -4.2220268 -2.9093304 1.7802717
C -4.4178398 -1.3135874 0.3200127
H -5.2687238 -0.8539484 0.8373437
C -3.1199658 -3.4271414 -0.0184443
H -3.0411468 -4.4874644 0.2503487
C -3.2996498 -3.2915594 -1.5376643
H -4.2076998 -3.8181574 -1.8594153
H -2.4530038 -3.7565134 -2.0598933
C -4.5946108 -1.1685834 -1.1973153
H -4.6734588 -0.1066544 -1.4664263
H -5.5245408 -1.6550154 -1.5196153
C -3.3906558 -1.8034104 -1.9056673
H -3.5033048 -1.6966894 -2.9913063
C -2.0996328 -1.0935774 -1.4707313
H -1.2557318 -1.5564454 -1.9969963
H -2.1244118 -0.0404694 -1.7721853
C -3.1290548 -0.6013504 0.7570497
H -3.0240058 -0.6970744 1.8419657

H -3.2071258 0.4712916 0.5368557
C -1.8322248 -2.7071044 0.4179047
H -1.6938108 -2.8237024 1.4996437
H -0.9692398 -3.1748154 -0.0705743
C -1.8906898 -1.2065464 0.0589157
E_{gas} = -1694.22005979
E_{THF} = -1694.25263188
G_{gas} = -1693.623375
G_{THF} = -1693.655947
Imaginary frequency = -387.4052

12b-anti

C -0.6787863 -0.2955042 -0.4547468
C 0.4423807 0.1018878 0.4820292
C -0.0366053 -0.0043622 1.9360252
C -1.3305083 -0.6460672 2.1630632
C -1.9304773 -1.4619712 1.2324752
C -1.5777263 -1.3035572 -0.1162378
H -0.5161193 -0.1208412 -1.5095108
H -1.7253093 -0.6081942 3.1739552
H -2.7808233 -2.0763832 1.5115502
H -2.1368333 -1.8061792 -0.8984178
C 0.6653717 0.3441318 3.0228542
H 1.6597737 0.7683008 2.9773792
H 0.2503507 0.1965108 4.0153072
B 1.4437107 -1.1264532 0.2213692
O 1.9652487 -1.9116272 1.2046612
O 1.8033077 -1.5255882 -1.0406058
C 2.4050257 -2.8325112 -0.9116238
C 2.8906167 -2.8302142 0.5806682
C 3.5101117 -2.9718172 -1.9472938
H 4.0290707 -3.9288992 -1.8273208
H 4.2408107 -2.1641442 -1.8674808
H 3.0778167 -2.9407162 -2.9515478
C 1.2928267 -3.8482612 -1.1793778
H 1.6708777 -4.8747692 -1.1530738
H 0.8713997 -3.6581772 -2.1705618
H 0.4861767 -3.7520322 -0.4453578
C 4.2922087 -2.2480322 0.7655412
H 4.4676277 -2.0862072 1.8326902
H 4.4008827 -1.2861132 0.2568382
H 5.0589677 -2.9310112 0.3868802
C 2.7883437 -4.1746422 1.2869012
H 3.4090547 -4.9221292 0.7809892
H 1.7582857 -4.5351252 1.3175302
H 3.1435677 -4.0761302 2.3166942
N -2.0681153 1.2094298 -0.1226768
N -2.3639493 1.3002788 1.1321582
C -3.2178713 0.7325638 -0.8746148
C -3.7214393 0.8736688 1.3248772
O -3.2586473 0.6114848 -2.0714198
O -4.3182963 0.8784388 2.3698462

N -4.2246823 0.5373558 0.0586112
C -5.5249253 0.0332518 -0.2141838
C -6.6175383 0.4948688 0.5187512
C -5.6946983 -0.9304762 -1.2082418
C -7.8810823 -0.0233132 0.2571642
H -6.4740973 1.2360818 1.2946022
C -6.9660773 -1.4292732 -1.4669588
H -4.8434723 -1.2702302 -1.7854378
C -8.0619053 -0.9829932 -0.7343348
H -8.7298533 0.3328078 0.8328042
H -7.0960983 -2.1753662 -2.2449418
H -9.0516873 -1.3811252 -0.9351828
C 2.7036947 1.3449208 0.4079862
H 2.8653847 1.1231168 1.4680312
H 3.1340417 0.5107978 -0.1613108
C 3.4650267 2.6235248 0.0299962
H 4.5213167 2.4991418 0.2988772
C 1.1895087 1.4586658 0.0837952
C 0.6221667 2.6994268 0.8114372
H 0.6840147 2.5744638 1.8957172
H -0.4366963 2.8131738 0.5695662
C 2.8712877 3.8205498 0.7848132
H 3.4227617 4.7359388 0.5324772
H 2.9731657 3.6698828 1.8679432
C 1.3901947 3.9697878 0.4104352
H 0.9589077 4.8217868 0.9494562
C 1.2630247 4.1997668 -1.1015528
H 0.2078007 4.3297188 -1.3728418
H 1.7904367 5.1179068 -1.3930668
C 3.3374407 2.8474878 -1.4824838
H 3.7787457 2.0013328 -2.0260118
H 3.8883827 3.7489598 -1.7812018
C 1.0796737 1.7249768 -1.4385798
H 1.4658387 0.8637438 -1.9997538
H 0.0280717 1.8645198 -1.7106898
C 1.8529387 2.9919508 -1.8419458
H 1.7466797 3.1338308 -2.9241628
E_{gas} = -1694.21294342
E_{THF} = -1694.24878357
G_{gas} = -1693.615643
G_{THF} = -1693.651484
Imaginary frequency = -270.2123

13a-syn

C -0.2292708 -1.5537043 -1.1363673
C -1.5067358 -1.5738173 -0.2365633
C -1.1116108 -2.3218303 1.0361397
C 0.3736262 -2.6330813 1.0712297
C 0.6720772 -3.5112624 -0.1279463
C 0.3463592 -2.9414033 -1.2910933
H -0.4083828 -1.0297423 -2.0735763
H 0.7084102 -3.0385583 2.0243607

H	1.1204702	-4.4923583	-0.0165903
H	0.4955042	-3.3933023	-2.2654943
C	-1.9511478	-2.7263163	1.9822397
H	-3.0172479	-2.5340994	1.9096697
H	-1.6003728	-3.2525403	2.8654397
B	-1.7865318	-0.0360923	0.0767697
O	-1.8025809	0.5195217	1.3210777
O	-1.9835638	0.8731917	-0.9283433
C	-2.2992139	2.1383817	-0.3061483
C	-1.7138108	1.9508937	1.1366947
C	-3.8218468	2.2741657	-0.3269993
H	-4.1433128	3.2432007	0.0671127
H	-4.2982478	1.4848537	0.2630897
H	-4.1726688	2.1847427	-1.3591053
C	-1.6552578	3.2526667	-1.1181603
H	-1.7825578	4.2178147	-0.6158133
H	-2.1310489	3.3153557	-2.1012483
H	-0.5897248	3.0695967	-1.2702513
C	-2.4994928	2.6403747	2.2418697
H	-2.0159779	2.4571997	3.2056297
H	-3.5241128	2.2668287	2.3004197
H	-2.5282658	3.7225207	2.0738907
C	-0.2303858	2.3126207	1.2340357
H	-0.0786748	3.3951057	1.1806697
H	0.3424252	1.8358297	0.4337467
H	0.1591302	1.9491787	2.1889077
N	0.7475282	-0.7470413	-0.3696073
N	1.0813352	-1.3485343	0.8697887
C	1.9038782	-0.2457233	-0.9471363
C	2.4470471	-1.2375783	1.0620447
O	1.9929462	0.2775007	-2.0339643
O	3.0849711	-1.7201493	1.9702927
N	2.9083181	-0.4297903	0.0117397
C	4.2353672	0.0683457	-0.1162773
C	5.3198282	-0.7076023	0.2895867
C	4.4334562	1.3416357	-0.6489643
C	6.6068862	-0.1947963	0.1658087
H	5.1543952	-1.6892013	0.7142437
C	5.7260812	1.8336337	-0.7821333
H	3.5837972	1.9309887	-0.9717123
C	6.8161892	1.0708657	-0.3726293
H	7.4506982	-0.7967183	0.4890267
H	5.8784402	2.8213727	-1.2060673
H	7.8238692	1.4621887	-0.4738283
C	-2.6449009	-2.2874644	-0.9566273
C	-3.3892288	-1.6568903	-2.1045643
H	-2.4813059	-3.3603623	-1.0384733
H	-3.6634019	-2.2969933	-2.9374423
H	-3.1389138	-0.6358903	-2.3729223
C	-4.0827238	-1.8729553	-0.7856553
H	-4.8356288	-2.6513854	-0.7114243
H	-4.2948838	-0.9933883	-0.1823933

$E_{\text{gas}} = -1421.45655186$

$E_{\text{THF}} = -1421.48944880$
 $G_{\text{gas}} = -1421.014848$
 $G_{\text{THF}} = -1421.047748$

13a-anti

C	-0.4533418	0.2764752	0.3523563
C	0.6332782	-0.8331548	0.4242963
C	0.2529982	-1.8732048	-0.6331937
C	-1.0043118	-1.4799448	-1.3839937
C	-0.7919918	-0.1001848	-1.9758837
C	-0.5064118	0.8275052	-1.0563537
H	-0.3112418	1.0328052	1.1236263
H	-1.3342218	-2.2352048	-2.0965537
H	-0.9021918	0.0871452	-3.0388137
H	-0.3434728	1.8798552	-1.2631737
C	0.9190282	-2.9958848	-0.8789937
H	1.8295382	-3.2394248	-0.3404837
H	0.5735982	-3.7033448	-1.6274437
B	2.0208082	-0.1514248	0.0711763
O	3.1182382	-0.8084048	-0.4132637
O	2.2354382	1.1917052	0.2530063
C	3.4920082	1.5048752	-0.3922537
C	4.2236282	0.1239952	-0.3690537
C	4.1862072	2.6105152	0.3845063
H	5.1798272	2.8054262	-0.0332637
H	4.2918872	2.3507352	1.4397163
H	3.5993172	3.5305352	0.3161363
C	3.1503372	1.9705852	-1.8060337
H	4.0450972	2.2791952	-2.3545637
H	2.4700772	2.8243352	-1.7402737
H	2.6484082	1.1754652	-2.3674037
C	4.9662782	-0.1307938	0.9406163
H	5.2825682	-1.1773538	0.9688963
H	4.3173082	0.0537652	1.8036763
H	5.8536782	0.5034062	1.0262763
C	5.1333582	-0.1357738	-1.5580637
H	5.9276482	0.6170762	-1.6050937
H	4.5754682	-0.1200038	-2.4961237
H	5.5992382	-1.1193938	-1.4540137
N	-1.7584218	-0.3757948	0.6190763
N	-2.0708618	-1.3623958	-0.3549137
C	-2.8849518	0.4151142	0.8206363
C	-3.3863418	-1.1742858	-0.7663337
O	-2.9482918	1.3986542	1.5191963
O	-3.9510418	-1.7741558	-1.6494137
N	-3.9092318	-0.1828658	0.0747163
C	-5.2731818	0.2239842	0.0764563
C	-6.2653118	-0.7385058	-0.1145937
C	-5.6076118	1.5641842	0.2689063
C	-7.5996718	-0.3500158	-0.1170137
H	-5.9878118	-1.7730658	-0.2768737
C	-6.9491828	1.9331442	0.2768663

H	-4.8273328	2.2977842	0.4248163
C	-7.9476618	0.9834942	0.0817163
H	-8.3703518	-1.0986968	-0.2706537
H	-7.2103628	2.9750642	0.4335963
H	-8.9916618	1.2806232	0.0841963
C	0.6523382	-1.4553748	1.8172463
C	1.3663782	-0.7563548	2.9397563
H	-0.2789418	-1.9536448	2.0748663
H	0.9074682	-0.7623948	3.9220863
H	1.8994582	0.1612052	2.7015963
C	1.9036282	-2.0527848	2.3932763
H	1.8007282	-2.9427748	3.0045563
H	2.8101482	-2.0220448	1.7962363

$E_{\text{gas}} = -1421.45551470$

$E_{\text{THF}} = -1421.48822271$

$G_{\text{gas}} = -1420.012029$

$G_{\text{THF}} = -1421.044741$

13b-syn

C	0.3300100	-1.1217099	-0.5593713
C	-0.7751970	-0.6118369	0.4317177
C	-0.3709770	-1.1847749	1.7968257
C	0.9224290	-1.9901089	1.7303857
C	0.7894780	-3.0860209	0.6978097
C	0.4798380	-2.6219179	-0.5145913
H	0.2068980	-0.7093199	-1.5574063
H	1.2556290	-2.3303379	2.7091807
H	0.9621830	-4.1278459	0.9436677
H	0.3644690	-3.2325889	-1.4039083
C	-0.9654170	-0.9917899	2.9707527
H	-1.8544930	-0.3831759	3.0849527
H	-0.5565170	-1.4243299	3.8797137
B	-0.5406030	0.9680841	0.4247957
O	-0.3188110	1.7441891	1.5240647
O	-0.4872350	1.6679311	-0.7516203
C	-0.3123340	3.0622601	-0.4255413
C	0.2218140	2.9973411	1.0502197
C	-1.6854670	3.7239071	-0.5449733
H	-1.6220780	4.8052341	-0.3881213
H	-2.3932350	3.3099671	0.1801167
H	-2.0809610	3.5414891	-1.5484493
C	0.6571260	3.6690611	-1.4303983
H	0.9065450	4.6996931	-1.1549743
H	0.1962770	3.6832691	-2.4223873
H	1.5767700	3.0840601	-1.4961863
C	-0.2638720	4.1180081	1.9579447
H	0.1543300	3.9839741	2.9596987
H	-1.3525990	4.1265921	2.0433257
H	0.0672550	5.0903131	1.5769757
C	1.7442900	2.8715461	1.1378497
H	2.2411620	3.8061871	0.8601117
H	2.1097900	2.0699611	0.4903377

H	2.0165650	2.6222061	2.1670247
N	1.5912600	-0.5350949	-0.0439443
N	1.9403020	-1.0385749	1.2309887
C	2.7363180	-0.4785669	-0.8254323
C	3.2914470	-1.3276299	1.2454757
O	2.7947850	-0.1463999	-1.9872603
O	3.9029950	-1.8605929	2.1436907
N	3.7881760	-0.8360199	0.0274567
C	5.1646920	-0.7777839	-0.3297043
C	6.0414890	-1.7755889	0.0931497
C	5.6233010	0.2916251	-1.0983133
C	7.3865590	-1.6893179	-0.2501453
H	5.6766570	-2.5944239	0.6996037
C	6.9668640	0.3550811	-1.4472543
H	4.9292610	1.0528991	-1.4332243
C	7.8536260	-0.6299109	-1.0214853
H	8.0710440	-2.4616479	0.0869947
H	7.3208370	1.1846801	-2.0515383
H	8.9041240	-0.5709179	-1.2893073
C	-5.0869690	-1.6735759	0.5284887
H	-6.1195640	-1.8836649	0.2203697
H	-5.0499150	-1.7673929	1.6218787
C	-4.6896210	-0.2512969	0.1089177
H	-5.3641040	0.4755191	0.5777167
C	-4.1238470	-2.6791689	-0.1178583
H	-4.3976730	-3.6977769	0.1828777
C	-4.2050800	-2.5527679	-1.6458943
H	-5.2237480	-2.7721549	-1.9917413
H	-3.5372100	-3.2840679	-2.1202443
C	-4.7650320	-0.1192689	-1.4179093
H	-4.4975380	0.9019221	-1.7206113
H	-5.7901950	-0.3026419	-1.7653283
C	-3.8018810	-1.1291599	-2.0563323
H	-3.8398220	-1.0337839	-3.1482303
C	-2.3642000	-0.8523259	-1.5870183
H	-1.7036690	-1.5840159	-2.0701643
H	-2.0429810	0.1435701	-1.9140823
C	-3.2523330	0.0344241	0.5684027
H	-3.2080460	-0.0062589	1.6614647
H	-2.9832520	1.0571781	0.2730927
C	-2.6869580	-2.3947539	0.3491797
H	-2.6206740	-2.5195729	1.4350907
H	-2.0090280	-3.1319569	-0.0940593
C	-2.2434580	-0.9683419	-0.0472993

$E_{\text{gas}} = -1694.29028040$

$E_{\text{THF}} = -1694.32538820$

$G_{\text{gas}} = -1693.687310$

$G_{\text{THF}} = -1693.722418$

13b-anti

C	-0.6404542	-0.7810943	-0.3613552
C	0.5030348	-0.1494253	0.4977308

C	0.1062238	-0.4318033	1.9549398	H	3.6545628	-3.7911403	1.4341198
C	-1.2503292	-1.1093183	2.0601298	H	4.9331308	-2.6858053	1.9548588
C	-1.1458932	-2.4158803	1.2987108	H	-6.1095992	0.5386987	1.5746208
C	-0.8152332	-2.2373213	0.0178148	H	-5.1117402	-1.5291673	-2.0506972
C	0.8416668	-0.2343823	3.0458518	H	-8.5114522	0.3763327	1.0092158
B	1.8024258	-0.9925283	0.1265748	H	-7.5135362	-1.6888863	-2.6205042
O	2.7920748	-1.3453283	0.9993258	H	-9.2255552	-0.7404993	-1.0917172
O	2.0078058	-1.4842533	-1.1388712	H	2.3958668	1.5951317	1.5885438
C	3.0780358	-2.4510003	-1.0489352	H	2.8940348	1.1661857	-0.0451552
C	3.8403398	-1.9836993	0.2397968	H	3.5209628	3.4852387	0.4760518
C	3.8962878	-2.4073493	-2.3306062	H	-0.0631152	2.1692997	2.0517028
C	2.4172328	-3.8213623	-0.8887772	H	-1.2442192	2.0972547	0.7492698
C	4.9096448	-0.9266873	-0.0398932	H	1.7330488	5.2118237	0.8025188
C	4.4290668	-3.1077583	1.0805878	H	1.6901388	4.0005407	2.0889628
N	-1.9000362	-0.0955423	-0.0137672	H	-0.6069702	4.4347087	1.2212788
N	-2.2360862	-0.2611373	1.3517788	H	-1.1759352	3.8220807	-1.1278502
C	-3.0408162	-0.2511053	-0.7791322	H	0.0418108	5.1027027	-1.1014392
C	-3.5912752	-0.5477273	1.4373088	H	2.9639568	2.8750557	-1.8755462
O	-3.0953522	-0.2319533	-1.9890562	H	2.4846528	4.5443577	-1.5458642
O	-4.1995462	-0.8380403	2.4417648	H	1.1822588	1.0236687	-1.9224252
N	-4.0920122	-0.3923443	0.1369588	H	-0.5040992	1.4627297	-1.6135202
C	-5.4707812	-0.4863283	-0.2046722	H	0.6612668	3.3073567	-2.7314362
C	-6.4230292	0.0598537	0.6550528	$E_{\text{gas}} = -1694.29124174$			
C	-5.8598582	-1.1213313	-1.3833262	$E_{\text{THF}} = -1694.3266658$			
C	-7.7712522	-0.0409413	0.3334738	$G_{\text{gas}} = -1693.687838$			
C	-7.2120422	-1.1998803	-1.6992132	$G_{\text{THF}} = -1693.723262$			
C	-8.1711042	-0.6669163	-0.8437292				
C	2.1947228	1.7864477	0.5288038				
C	2.4812928	3.2601077	0.2078408	14a			
C	0.7375368	1.3951247	0.1813838	C	-2.2528029	-0.7534548	-1.3023973
C	-0.2011682	2.3320977	0.9778578	C	-1.6851039	-0.0458208	-0.1540143
C	1.5293338	4.1537477	1.0137038	C	-2.2825449	-0.4090168	1.1419217
C	0.0810148	3.8058447	0.6434748	C	-3.6319999	-0.7915808	1.2284177
C	-0.1362042	4.0469327	-0.8574482	C	-4.1868609	-1.2844718	0.0669957
C	2.2703138	3.4974457	-1.2940352	C	-3.4722069	-1.3461538	-1.1739123
C	0.5308878	1.6782077	-1.3264482	H	-1.7491429	-0.7109238	-2.2648683
C	0.8208608	3.1511827	-1.6579062	H	-4.1499809	-0.8746038	2.1794017
H	-0.4804982	-0.6463763	-1.4267042	H	-5.1825609	-1.7201618	0.1039997
H	-1.5976962	-1.2123543	3.0865618	H	-3.9468579	-1.8346258	-2.0194923
H	-1.3483312	-3.3712543	1.7700768	C	-1.1800099	-0.3424698	2.0382817
H	-0.7099802	-3.0277563	-0.7167102	H	-1.2991369	-0.0236378	3.0768407
H	1.8559498	0.1439927	3.0011998	H	-0.6300089	-1.2874628	1.9866447
H	0.4486928	-0.4686313	4.0316318	B	-0.0900959	-0.1330898	0.4804257
H	4.7584748	-3.0790103	-2.2570942	O	0.8306841	0.9198452	0.3467807
H	4.2547878	-1.3986553	-2.5455542	O	0.5872011	-1.3619578	0.2351357
H	3.2798048	-2.7347673	-3.1727712	C	1.8666951	-1.0550628	-0.3104873
H	3.1600888	-4.6242923	-0.8652672	C	2.1453441	0.3614462	0.2860287
H	1.7488638	-3.9934253	-1.7376722	C	1.7324261	-1.0340628	-1.8379503
H	1.8207408	-3.8670173	0.0279918	H	2.6973871	-0.8852608	-2.3338723
H	5.2172318	-0.4754673	0.9075848	H	1.0494421	-0.2400148	-2.1585303
H	4.5305968	-0.1308793	-0.6873062	H	1.3167061	-1.9917468	-2.1653993
H	5.7894828	-1.3691903	-0.5171872	C	2.8606881	-2.1307348	0.1094027
H	5.1649918	-3.6771373	0.5025348	H	3.8765561	-1.8701588	-0.2092773

H	2.5921161	-3.0844598	-0.3553363
H	2.8576951	-2.2703738	1.1927837
C	3.0215951	1.2616362	-0.5759313
H	3.1551271	2.2304242	-0.0847463
H	2.5691841	1.4386812	-1.5545693
H	4.0107231	0.8132202	-0.7230653
C	2.6970051	0.3044992	1.7137717
H	3.7357121	-0.0415258	1.7334857
H	2.0942021	-0.3604388	2.3399067
H	2.6560771	1.3076182	2.1483247
C	-2.0573989	1.4609652	-0.3654303
C	-1.2134489	2.4533652	-1.1145133
H	-3.1273049	1.5449402	-0.5530823
H	-1.7150049	3.0947942	-1.8335553
H	-0.2015789	2.1621212	-1.3719463
C	-1.4781469	2.6411562	0.3584967
H	-2.1819109	3.4066892	0.6723717
H	-0.6384609	2.4818692	1.0229577

$E_{\text{gas}} = -798.800067942$

$E_{\text{THF}} = -798.815603692$

$G_{\text{gas}} = -798.521084$

$G_{\text{THF}} = -798.536620$

Imaginary frequency = -565.2303

C	3.1081406	1.1939321	-0.4468414
H	3.2668686	2.1322231	0.1069196
H	2.7269126	1.4201791	-1.4489074
H	4.0979246	0.7442611	-0.5670454
C	2.6214336	0.1388091	1.7749656
H	3.6377266	-0.2590749	1.8409646
H	1.9550626	-0.5193989	2.3381316
H	2.6111766	1.1229191	2.2556686
C	-2.1472834	1.4020631	-0.3990154
C	-1.2706164	2.3559451	-1.1514944
H	-3.2150734	1.4903381	-0.5822144
H	-1.7405024	3.0753781	-1.8135774
H	-0.3497084	1.9294551	-1.5487414
C	-1.5319164	2.5401561	0.3521786
H	-2.1788584	3.3682391	0.6209716
H	-0.8288994	2.2625391	1.1362206
Li	0.8087706	2.6798601	-0.0213084

$E_{\text{gas}} = -806.190374218$

$E_{\text{THF}} = -806.272796603$

$E_{\text{CHCl}_3} = -806.268853636$

$G_{\text{gas}} = -805.866991$

$G_{\text{THF}} = -805.949414$

$G_{\text{CHCl}_3} = -805.945470$

Imaginary frequency = -544.5417

14a_{Li}⁺

C	-2.3113284	-0.8133499	-1.3204874
C	-1.7104704	-0.0829939	-0.1868044
C	-2.2866314	-0.4406259	1.1368606
C	-3.6510544	-0.7606359	1.2496686
C	-4.2343084	-1.2520679	0.1028966
C	-3.5423244	-1.3598689	-1.1549014
H	-1.8156684	-0.8247759	-2.2874104
H	-4.1553104	-0.8215409	2.2086656
H	-5.2402694	-1.6590929	0.1626486
H	-4.0442024	-1.8606669	-1.9760564
C	-1.1728524	-0.3995859	2.0092496
H	-1.2740924	-0.1437679	3.0658586
H	-0.6113914	-1.3351919	1.9004166
B	-0.1283684	-0.1911459	0.3961936
O	0.8531676	0.8780861	0.3147206
O	0.5556066	-1.3830779	0.1055726
C	1.8763776	-1.1028089	-0.3592944
C	2.1742006	0.2666541	0.3212506
C	1.8244206	-1.0079819	-1.8870594
H	2.8170896	-0.8662419	-2.3255084
H	1.1750086	-0.1878989	-2.2160604
H	1.4073086	-1.9387449	-2.2795944
C	2.8074866	-2.2288139	0.0680676
H	3.8478396	-1.9953519	-0.1828114
H	2.5319586	-3.1487189	-0.4540524
H	2.7366516	-2.4176159	1.1410976

14a_{LiB(CH₃)₄}

C	3.5754591	-0.7289251	-1.2919045
C	2.5919541	-0.8187151	-0.2076615
C	3.1691282	-1.0738651	1.1280355
C	4.3372322	-1.8429481	1.2613935
C	5.1491742	-1.8887821	0.1484985
C	4.8114672	-1.2622721	-1.0972925
H	3.2810022	-0.3284321	-2.2584705
H	4.6774661	-2.2187541	2.2215425
H	6.1276952	-2.3549171	0.2340465
H	5.5514991	-1.2622261	-1.8911325
C	2.3152962	-0.3414881	1.9992205
H	2.0838561	-0.6947391	3.0068915
H	2.6574042	0.6979079	2.0283695
B	1.5873372	0.4224699	0.3922295
O	0.1723632	0.5405119	0.1809055
O	2.1603602	1.7051599	0.2238665
C	1.1732222	2.5888459	-0.2963215
C	-0.1417298	1.9636829	0.2478515
C	1.2604732	2.5447009	-1.8264365
H	0.5934402	3.2738889	-2.2966845
H	1.0090322	1.5490949	-2.2081675
H	2.2885562	2.7729359	-2.1225525
C	1.4543512	4.0008119	0.2013205
H	0.6498292	4.6851439	-0.0895435
H	2.3869041	4.3664399	-0.2388265

H	1.5618342	4.0243219	1.2879255
C	-1.3724338	2.2549389	-0.5922755
H	-2.2633529	1.8084749	-0.1436395
H	-1.2735018	1.8673889	-1.6085475
H	-1.5340478	3.3368519	-0.6489385
C	-0.4037758	2.3181949	1.7117635
H	-0.6926868	3.3687819	1.8121605
H	0.4810152	2.1407519	2.3301205
H	-1.2225788	1.7046029	2.0945625
C	1.7519452	-2.1010841	-0.4997685
C	0.4513872	-2.0452091	-1.2448415
H	2.3943882	-2.9530061	-0.7129665
H	0.2260222	-2.8362681	-1.9521405
H	0.1041722	-1.0626931	-1.5490605
C	0.4856422	-2.4187721	0.2253915
H	0.2957762	-3.4573751	0.4731085
H	0.1635422	-1.7238491	0.9962655
Li	-1.4644128	-0.7213201	-0.0189725
C	-5.2442049	-1.1577541	0.0708715
H	-5.6302328	-1.6565511	0.9720465
H	-5.6724809	-0.1437411	0.0623805
H	-5.6717919	-1.6884701	-0.7924795
C	-3.0460429	-2.6978111	0.0988615
H	-3.3371269	-3.1786281	1.0436645
H	-3.4872249	-3.2894401	-0.7156355
H	-1.9575798	-2.8593731	0.0072155
C	-3.1978189	-0.4544031	-1.4460215
H	-3.6563199	-1.0952211	-2.2099295
H	-3.6400169	0.5442829	-1.5615825
H	-2.1513129	-0.3431291	-1.8080965
C	-3.1263759	-0.3060221	1.4133005
H	-2.0743119	-0.2896361	1.7733975
H	-3.4499908	0.7451869	1.4030925
H	-3.6560979	-0.7847771	2.2461095
B	-3.6127769	-1.1447721	0.0334805

$E_{\text{gas}} = -990.923080058$

$E_{\text{THF}} = -990.947834638$

$E_{\text{CHCl}_3} = -990.950052782$

$G_{\text{gas}} = -990.455254$

$G_{\text{THF}} = -990.480009$

$G_{\text{CHCl}_3} = -990.482227$

Imaginary frequency = -560.2586

14a_{Li(THF)₂⁺}

C	-3.6521601	-0.5735194	1.8317433
C	-2.6462021	-0.8251084	0.7859653
C	-3.1188711	-1.7010114	-0.3119957
C	-4.0359841	-2.7327464	-0.0542017
C	-4.8307671	-2.5518024	1.0570943
C	-4.6979221	-1.4327454	1.9485273

H	-3.4972401	0.2240596	2.5534933
H	-4.2515041	-3.5117824	-0.7786217
H	-5.6518971	-3.2427024	1.2300603
H	-5.4326531	-1.3140374	2.7379793
B	-1.9852191	0.2978846	-0.2953347
O	-0.6282001	0.7777006	-0.2605397
O	-2.8121811	1.4080846	-0.5615197
C	-2.0614991	2.6087406	-0.3964867
C	-0.6246571	2.1409746	-0.7686617
C	-2.1755881	3.0449786	1.0681833
H	-1.6863251	4.0073866	1.2475713
H	-1.7373651	2.3003976	1.7426173
H	-3.2347071	3.1470066	1.3192473
C	-2.6326681	3.6835206	-1.3110507
H	-2.0121201	4.5861496	-1.2921697
H	-3.6360701	3.9554536	-0.9723537
H	-2.7111461	3.3288406	-2.3408247
C	0.5050019	2.8996316	-0.0857627
H	1.4770389	2.5457666	-0.4522587
H	0.4742379	2.7810246	1.0007243
H	0.4466189	3.9671726	-0.3195927
C	-0.3833491	2.0843166	-2.2756177
H	-0.3376531	3.0890136	-2.7053187
H	-1.1743151	1.5250686	-2.7836027
H	0.5741769	1.5932576	-2.4752027
C	-1.5340331	-1.6632214	1.4944153
C	-0.3063861	-1.0336484	2.0773003
H	-1.9640031	-2.4822874	2.0662173
H	0.0525249	-1.4128804	3.0288153
H	-0.1815761	0.0366156	1.9469263
C	-0.2036071	-1.9607864	0.8757333
H	0.2114119	-2.9504984	1.0392753
H	-0.0360531	-1.5787644	-0.1253007
Li	1.1323869	0.1266686	0.1149443
C	3.0414189	-0.4495484	2.3098653
O	2.5953319	0.4879576	1.3129943
C	3.6949639	1.3196586	0.8839883
C	4.8966799	0.9007746	1.7311963
C	4.5478679	-0.5391394	2.1198333
H	2.7785269	-0.0641734	3.3017593
H	2.5105699	-1.3902944	2.1431423
H	3.8539129	1.1354906	-0.1848317
H	3.4151049	2.3662456	1.0267273
H	5.8368019	0.9829236	1.1820853
H	4.9705049	1.5275496	2.6251273
H	4.7910349	-1.2316744	1.3069503
H	5.0617489	-0.8762604	3.0223333
C	2.9507329	-1.6975864	-1.1608337
O	1.9329389	-0.7131284	-1.4289547
C	1.1262689	-1.1272884	-2.5524507
C	1.3463659	-2.6276254	-2.6597287
C	2.8188259	-2.7543064	-2.2569057
H	3.9236279	-1.1990944	-1.1512077

H	2.7596199	-2.1203324	-0.1664137
H	0.0950209	-0.8368914	-2.3399227
H	1.4747549	-0.6002424	-3.4479627
H	0.7013939	-3.1605364	-1.9519587
H	1.1427789	-3.0085364	-3.6626407
H	3.0856909	-3.7518034	-1.9015967
H	3.4668169	-2.5096714	-3.1041967
C	-2.4953851	-1.1580194	-1.4672297
H	-2.2283571	-1.7897084	-2.3187507
H	-3.0950391	-0.3069104	-1.8108337

$E_{\text{gas}} = -1271.18631888$

$E_{\text{THF}} = -1271.25683877$

$E_{\text{CHCl}_3} = -1271.25633339$

$G_{\text{gas}} = -1270.639005$

$G_{\text{THF}} = -1270.709369$

$G_{\text{CHCl}_3} = -1270.709020$

Imaginary frequency = -540.2805

H	-3.8883275	-1.5150332	-1.2018323
H	-4.3516835	0.0988248	-1.7577323
C	2.4205085	1.7272728	-0.5860693
C	2.5668965	2.7800128	0.4781807
H	2.5890865	2.0763788	-1.6047253
H	2.8795085	3.7744028	0.1746427
H	2.9355095	2.4724578	1.4523377
C	1.1951785	2.3068478	0.0816617
H	0.5620665	2.9715388	-0.4997133
H	0.6673725	1.6638258	0.7794397

$E_{\text{gas}} = -798.945536508$

$E_{\text{THF}} = -798.964116502$

$E_{\text{CHCl}_3} = -798.966060073$

$G_{\text{gas}} = -798.624222$

$G_{\text{THF}} = -798.642907$

$G_{\text{CHCl}_3} = -798.644745$

15a

C	3.9502435	0.0128688	0.4301947
C	2.8299675	0.3060528	-0.3486073
C	2.1085535	-0.7479682	-0.9372333
C	2.5268215	-2.0595772	-0.7088493
C	3.6372475	-2.3418282	0.0794907
C	4.3562885	-1.2989642	0.6516827
H	4.5150135	0.8323058	0.8665107
H	1.9670905	-2.8767132	-1.1587283
H	3.9391745	-3.3725902	0.2417857
H	5.2312125	-1.5026542	1.2621587
C	0.8812455	-0.4876332	-1.7746323
H	0.7504755	-1.2947462	-2.5081113
H	0.9866025	0.4286938	-2.3669513
B	-0.4582805	-0.3833502	-0.9491883
O	-1.6694545	-0.1152682	-1.5343213
O	-0.5517855	-0.5751332	0.4040607
C	-1.9523075	-0.6415862	0.7371777
C	-2.6238365	0.0981508	-0.4736043
C	-2.1665995	0.0211118	2.0909547
H	-3.2335215	0.0594618	2.3368777
H	-1.7667635	1.0374388	2.1072207
H	-1.6561525	-0.5554872	2.8678037
C	-2.3142955	-2.1260252	0.8152027
H	-3.3532205	-2.2721002	1.1269997
H	-1.6594435	-2.6099432	1.5451677
H	-2.1671605	-2.6201832	-0.1502903
C	-2.7324765	1.6107558	-0.2722253
H	-3.0199085	2.0734148	-1.2206173
H	-1.7746365	2.0404938	0.0363997
H	-3.4861975	1.8632658	0.4800307
C	-3.9704605	-0.4679402	-0.9033383
H	-4.6995515	-0.3908532	-0.0892103

16

C	-0.9978714	0.8471089	1.9812664
C	-0.7059334	0.5876289	0.5215564
C	-0.7342864	1.8773309	-0.3354136
C	-1.2722374	3.0929099	0.2756884
C	-1.5915964	3.1650239	1.5783374
C	-1.4093264	2.0231569	2.4647124
H	-0.8582624	0.0108119	2.6617484
H	-1.4159584	3.9655379	-0.3530956
H	-1.9864024	4.0893229	1.9909754
H	-1.6063404	2.1462359	3.5258704
C	-0.3028674	1.8397589	-1.6131416
H	0.0864006	0.8939489	-1.9887546
B	0.7843956	0.0644519	0.3964944
O	1.2038366	-0.8168651	-0.5699886
O	1.8055376	0.4997209	1.1980434
C	3.0363906	0.1115689	0.5537224
C	2.5873026	-1.1242591	-0.2971636
C	4.0812496	-0.1871491	1.6184834
H	5.0000266	-0.5681801	1.1591264
H	3.7192656	-0.9221811	2.3405034
H	4.3252196	0.7303189	2.1617804
C	3.4740666	1.3016889	-0.3026506
H	4.4367736	1.1170599	-0.7896116
H	3.5712676	2.1800709	0.3413434
H	2.7264426	1.5301279	-1.0692266
C	2.6007296	-2.4338651	0.4930264
H	2.0751236	-3.2003121	-0.0840046
H	2.0879006	-2.3200541	1.4534234
H	3.6217156	-2.7803271	0.6813624
C	3.3202186	-1.2964851	-1.6194766
H	4.3916416	-1.4489441	-1.4493836
H	3.1876586	-0.4263111	-2.2658836

H	2.9296956	-2.1729841	-2.1447816
C	-1.7196124	-0.4565401	-0.0586856
C	-1.6743694	-1.8151561	0.6577714
C	-3.1585664	0.0760899	-0.0858126
H	-1.4101994	-0.6335271	-1.0985486
C	-2.6217774	-2.8222441	-0.0008326
H	-1.9725064	-1.6923961	1.7079594
H	-0.6513334	-2.2095311	0.6544234
C	-4.1232144	-0.9284851	-0.7229146
H	-3.4786554	0.2930879	0.9428664
H	-3.1930064	1.0239969	-0.6333816
C	-4.0573174	-2.2923471	-0.0312966
H	-2.5796914	-3.7809851	0.5296024
H	-2.2842594	-3.0142511	-1.0291966
H	-5.1463334	-0.5351711	-0.6928346
H	-3.8651804	-1.0525501	-1.7844896
H	-4.7182674	-3.0081221	-0.5344536
H	-4.4251814	-2.1912751	0.9998284
C	-0.2843364	2.9516749	-2.6202166
H	0.7404606	3.1376509	-2.9665996
H	-0.8694854	2.6776229	-3.5071356
H	-0.6789454	3.8965899	-2.2409416

$E_{\text{gas}} = -956.191635785$

$E_{\text{THF}} = -956.210354904$

$G_{\text{gas}} = -955.757532$

$G_{\text{THF}} = -955.776240$

17a-syn

C	0.3538699	-0.8553074	-0.7724123
C	-0.8236631	-0.7289034	0.1597677
C	-0.4717361	-1.2285304	1.5648167
C	0.8805729	-1.7767414	1.7444227
C	1.5875439	-2.3104684	0.6599457
C	1.3439909	-1.7946284	-0.6200843
H	0.2981109	-0.2925214	-1.6994073
H	1.1700129	-2.0996964	2.7365517
H	2.4430569	-2.9508714	0.8464627
H	2.0457609	-1.9889124	-1.4263493
C	-1.3478911	-1.1663154	2.5793627
H	-2.3189871	-0.7243544	2.3690487
B	-1.2167651	0.8149076	0.1881237
O	-1.8745761	1.4273056	1.2198207
O	-1.0677481	1.6216306	-0.9079853
C	-1.4102611	2.9613356	-0.4965313
C	-2.3639441	2.6904996	0.7181567
C	-2.0602181	3.6796596	-1.6701303
H	-2.4193761	4.6685846	-1.3645453
H	-2.9006201	3.1111536	-2.0751453
H	-1.3237721	3.8152586	-2.4674023
C	-0.1093341	3.6581936	-0.0994023
H	-0.2815951	4.7137526	0.1350967

H	0.5970629	3.5862636	-0.9302413
H	0.3525099	3.1685846	0.7620777
C	-3.8184411	2.4591226	0.3041927
H	-4.3770561	2.0853166	1.1672397
H	-3.8876561	1.7124376	-0.4938953
H	-4.2913881	3.3833786	-0.0417063
C	-2.2899301	3.7247796	1.8312827
H	-2.5711261	4.7139786	1.4535207
H	-1.2857431	3.7830106	2.2551647
H	-2.9837241	3.4554046	2.6333147
C	2.5793449	0.9137246	-0.1557883
C	3.2716839	-0.3746554	1.5731117
O	2.5800459	1.6188166	-1.1322293
O	3.9249009	-1.0050004	2.3638657
C	-2.0475991	-1.5424514	-0.4214663
C	-2.4756781	-1.1082614	-1.8328443
C	-1.8374171	-3.0629654	-0.3959613
H	-2.8859651	-1.3184314	0.2554197
C	-3.7499351	-1.8366604	-2.2705743
H	-1.6724111	-1.3436334	-2.5452333
H	-2.6214231	-0.0247264	-1.8826173
C	-3.1035021	-3.8063114	-0.8330723
H	-1.0110931	-3.3261244	-1.0702313
H	-1.5436151	-3.3849794	0.6084837
C	-3.5700121	-3.3554774	-2.2191463
H	-4.0313321	-1.5201874	-3.2816633
H	-4.5768121	-1.5460514	-1.6065613
H	-2.9230461	-4.8875744	-0.8247863
H	-3.9023411	-3.6148954	-0.1023663
H	-4.5041641	-3.8606304	-2.4908153
H	-2.8197871	-3.6529494	-2.9653663
C	-1.1658741	-1.5992924	4.0016007
H	-0.2028611	-2.0715324	4.2050927
H	-1.2583051	-0.7327954	4.6672847
H	-1.9535171	-2.3058774	4.2896907
N	1.4742119	0.6873046	0.7195357
N	1.8664999	-0.0320164	1.7278757
N	3.6771659	0.2337656	0.3962207
C	4.9766759	0.1531446	-0.1719093
C	5.6797759	-1.0488684	-0.1047113
C	5.5340779	1.2673846	-0.7967303
C	6.9504919	-1.1302794	-0.6619193
H	5.2411359	-1.9050834	0.3934827
C	6.8009269	1.1674766	-1.3614183
H	4.9734539	2.1920526	-0.8533243
C	7.5137999	-0.0259534	-1.2945623
H	7.4984769	-2.0656204	-0.6030733
H	7.2332449	2.0340856	-1.8519903
H	8.5038379	-0.0957744	-1.7344363

$E_{\text{gas}} = -1578.68715526$

$E_{\text{THF}} = -1578.71962664$

$G_{\text{gas}} = -1578.136954$

$G_{\text{THF}} = -1578.169426$

Imaginary frequency = -388.4938

17b-syn

C	-0.3473319	-1.0570975	-1.7451282
C	-0.7233929	-0.7203445	-0.3047892
C	-0.2422469	-1.8155605	0.6569658
C	0.2207431	-3.0547355	0.0401418
C	-0.0222359	-3.3867155	-1.2671462
C	-0.3410349	-2.3714975	-2.1882512
H	-0.5422269	-0.2811045	-2.4768772
H	0.6419651	-3.8164235	0.6882808
H	0.2033481	-4.3884015	-1.6194822
H	-0.3603419	-2.5783045	-3.2544012
C	-0.3010609	-1.6642565	1.9937818
H	-0.6588159	-0.7124315	2.3759328
B	-0.1239259	0.7052665	0.0638318
O	-0.0722319	1.2171685	1.3329698
O	0.3078151	1.5992385	-0.8804792
C	0.9272631	2.7003685	-0.1857912
C	0.2565901	2.6173905	1.2293888
C	0.6494091	3.9816325	-0.9572592
H	1.0482131	4.8493715	-0.4205562
H	-0.4203649	4.1292585	-1.1191542
H	1.1351471	3.9297125	-1.9357232
C	2.4292231	2.4124495	-0.1593832
H	2.9864641	3.2300595	0.3085458
H	2.7782121	2.3010065	-1.1902252
H	2.6431561	1.4833625	0.3797188
C	-1.0614279	3.3874085	1.3225378
H	-1.5569539	3.1292095	2.2628198
H	-1.7356489	3.1222565	0.5020918
H	-0.8967869	4.4691075	1.3022848
C	1.1675821	2.9898565	2.3904488
H	1.5141361	4.0243595	2.2920308
H	2.0363601	2.3299315	2.4392268
H	0.6201291	2.9010185	3.3334798
C	1.9732001	-0.0842455	-2.9649662
C	3.0349221	-1.9280385	0.2761888
O	1.1763841	0.1617305	-3.8345672
O	3.7473901	-2.9105335	0.2368148
C	-2.2911899	-0.5655535	-0.1870212
C	-2.8752999	0.4874565	-1.1444152
C	-3.0770539	-1.8759285	-0.3282952
H	-2.4584789	-0.2041815	0.8394338
C	-4.3624069	0.7249525	-0.8695932
H	-2.7603179	0.1421045	-2.1803702
H	-2.3231859	1.4323005	-1.0758512
C	-4.5692939	-1.6550255	-0.0587232
H	-2.9456219	-2.2759055	-1.3425852
H	-2.6820479	-2.6263735	0.3639618
C	-5.1564479	-0.5792295	-0.9751312
H	-4.7570949	1.4694365	-1.5709172

H	-4.4827589	1.1449275	0.1395198
H	-5.1123219	-2.5990785	-0.1842152
H	-4.7047589	-1.3510445	0.9891068
H	-6.2119799	-0.4052695	-0.7356002
H	-5.1216539	-0.9352945	-2.0145772
C	0.0875891	-2.6478705	3.0565278
H	0.8113041	-2.1913775	3.7434618
H	-0.7831889	-2.9289585	3.6628218
H	0.5317621	-3.5692645	2.6728378
O	2.9227771	-1.1181785	1.3538678
O	3.2344431	0.3695225	-3.1008962
C	2.2125831	-1.4462865	-0.7817862
C	1.6688161	-0.8732685	-1.7473912
C	4.3042591	-0.0165725	-2.2453022
H	4.1668471	0.3726585	-1.2333372
H	4.4170561	-1.1033825	-2.2090372
H	5.1928021	0.4306915	-2.6923782
C	3.6313691	-1.5534345	2.5106048
H	3.4373121	-0.7968405	3.2707398
H	3.2621031	-2.5274525	2.8432328
H	4.7024571	-1.6297555	2.3080068

$E_{\text{gas}} = -1489.23387813$

$E_{\text{THF}} = -1489.26112583$

$G_{\text{gas}} = -1488.693693$

$G_{\text{THF}} = -1488.720940$

Imaginary frequency = -358.1324

17c-syn

C	-1.4732112	0.4546176	-1.2308726
C	-0.5390622	0.4981376	-0.0269406
C	-1.3510482	0.6617556	1.2664044
C	-2.7789802	0.9577796	1.0800604
C	-3.2427202	1.5637546	-0.0815076
C	-2.5711222	1.3109156	-1.2760786
H	-1.0307512	0.1326326	-2.1694096
H	-3.4076572	1.0040146	1.9627104
H	-4.2228892	2.0297796	-0.0913276
H	-3.0290672	1.5655046	-2.2271396
C	-0.7818672	0.5991536	2.4828524
H	0.2808918	0.3766706	2.5289784
B	0.4206308	-0.7689334	0.0042204
O	1.2559578	-1.0692234	1.0458374
O	0.5758648	-1.6259344	-1.0556276
C	1.4378438	-2.7049054	-0.6270696
C	2.1998518	-2.0585564	0.5819294
C	2.3203588	-3.1166934	-1.7957926
H	3.0429078	-3.8774354	-1.4814926
H	2.8645168	-2.2636554	-2.2065256
H	1.7023378	-3.5402364	-2.5924516
C	0.5239468	-3.8603664	-0.2173586
H	1.0989628	-4.7423074	0.0803654

H -0.1075572 -4.1338274 -1.0679036
H -0.1300372 -3.5744404 0.6131704
C 3.4634278 -1.3008554 0.1719594
H 3.8231628 -0.7254514 1.0295694
H 3.2628668 -0.5996004 -0.6438156
H 4.2561138 -1.9856884 -0.1437266
C 2.5105618 -3.0136244 1.7254034
H 3.1621598 -3.8242004 1.3818544
H 1.6010798 -3.4478404 2.1452224
H 3.0290068 -2.4755284 2.5243174
C -3.6124182 -1.2811944 -1.8102816
C -4.6047512 -1.0374514 0.2118984
O -3.5570682 -1.4241874 -2.9981566
O -5.5238332 -0.9382674 0.9743964
C 0.4645898 1.7183036 -0.1819206
C 1.2591968 1.6806516 -1.4984856
C -0.1543522 3.1103866 -0.0043096
H 1.1839248 1.5865776 0.6404804
C 2.3587508 2.7458006 -1.5116576
H 0.5754768 1.8667456 -2.3378956
H 1.6924368 0.6882166 -1.6728286
C 0.9331058 4.1908266 -0.0112246
H -0.8660102 3.3056946 -0.8162736
H -0.7186872 3.1554326 0.9325844
C 1.7723628 4.1422856 -1.2903506
H 2.9052818 2.7076016 -2.4610886
H 3.0860088 2.5241956 -0.7173416
H 0.4739218 5.1794006 0.1041434
H 1.5906338 4.0458576 0.8578814
H 2.5720228 4.8908186 -1.2514496
H 1.1360268 4.4024486 -2.1479876
C -1.4286372 0.8062396 3.8205834
H -0.9520172 1.6418196 4.3482024
H -2.4992252 1.0155206 3.7708114
H -1.2911862 -0.0809654 4.4507984
O -4.7929042 -0.9583804 -1.1665236
C -2.5453152 -1.3744804 -0.7827906
H -1.6523172 -1.9422874 -1.0018816
C -3.1666922 -1.2349774 0.4513754
H -2.8048042 -1.5780464 1.4094754

$E_{\text{gas}} = -1335.45975502$

$E_{\text{THF}} = -1335.48975266$

$G_{\text{gas}} = -1334.972635$

$G_{\text{THF}} = -1335.002633$

Imaginary frequency = -517.0099

17d-syn

C 1.0955874 -0.3671143 -1.6338687
C 0.3730504 -0.6445173 -0.3118507
C 1.4201534 -0.9842333 0.7529453
C 2.6694504 -1.5442223 0.2168293
C 2.8005004 -1.9485393 -1.1065917

C 2.0263824 -1.3093293 -2.0703627
H 0.5381524 0.1964767 -2.3776697
H 3.3987814 -1.9150853 0.9300853
H 3.6501724 -2.5537763 -1.4024967
H 2.2915634 -1.3827263 -3.1206467
C 1.2106344 -0.8483683 2.0746883
H 0.2829604 -0.3857513 2.3926463
B -0.6950866 0.4830177 0.0573163
O -1.2340856 0.6507897 1.3051293
O -1.3656256 1.2151327 -0.8990777
C -2.5678526 1.7359907 -0.2879417
C -2.2273506 1.6908977 1.2442413
C -3.7116846 0.7991497 -0.6848847
H -4.6730266 1.1628807 -0.3090797
H -3.5530636 -0.2138433 -0.3043027
H -3.7642376 0.7444537 -1.7763517
C -2.8571666 3.1304897 -0.8244837
H -3.7743536 3.5251397 -0.3737827
H -3.0046476 3.0856737 -1.9081777
H -2.0461316 3.8269377 -0.6095477
C -3.3930226 1.2935597 2.1418323
H -3.0570506 1.2649617 3.1824713
H -3.7864526 0.3069447 1.8875723
H -4.2037016 2.0265247 2.0666053
C -1.5792466 2.9714627 1.7697093
H -2.3023666 3.7925847 1.8113733
H -0.7248646 3.2613847 1.1541603
H -1.2114416 2.7853807 2.7830123
C 1.6841064 2.2179687 -0.9248207
C 4.7848234 0.1718667 -0.5426167
O 1.1881674 2.4798917 0.1537023
O 5.1045564 -0.0732113 -1.6856177
C -0.4857486 -1.9834453 -0.5547737
C -1.3612766 -2.3824073 0.6421143
C -1.3318006 -1.9650263 -1.8391457
H 0.2623804 -2.7780453 -0.6804447
C -2.0364436 -3.7364163 0.4101373
H -2.1379176 -1.6267953 0.8138043
H -0.7579296 -2.4150863 1.5540823
C -2.0353356 -3.3075803 -2.0658187
H -2.0778596 -1.1639453 -1.7869697
H -0.7018346 -1.7461683 -2.7066907
C -2.8851736 -3.7158033 -0.8620197
H -2.6528246 -3.9974343 1.2786493
H -1.2685116 -4.5178443 0.3212723
H -2.6521536 -3.2531903 -2.9707497
H -1.2769416 -4.0822633 -2.2479977
H -3.3492706 -4.6941093 -1.0336107
H -3.7045826 -2.9928573 -0.7360197
C 2.1295344 -1.2408893 3.1950533
H 2.9378994 -1.9131303 2.8953663
H 2.5837344 -0.3514323 3.6535063
H 1.5656184 -1.7433903 3.9893603

C	2.6268514	1.1169517	-1.1965857
H	3.0477664	1.1175797	-2.1944187
C	3.4431854	0.6508217	-0.1676597
H	3.2125074	0.9487787	0.8459423
C	5.4355444	0.3245477	1.7760483
H	6.3402914	0.0770177	2.3328603
H	4.5936414	-0.2362383	2.1956553
H	5.2405294	1.3983567	1.8709993
C	0.5112754	3.9762127	-1.9744327
H	0.7612314	4.6588077	-2.7869837
H	0.5744474	4.4856577	-1.0105757
H	-0.4919356	3.5712627	-2.1152697
O	1.4528624	2.9119117	-2.0486877
O	5.7016544	-0.0432533	0.4338523

$E_{\text{gas}} = -1490.50086817$

$E_{\text{THF}} = -1490.52692290$

$G_{\text{gas}} = -1489.931204$

$G_{\text{THF}} = -1489.957259$

Imaginary frequency = -472.6604

17e-syn

C	0.7598965	-0.7825430	-1.2359209
C	-0.2326345	-0.7355700	-0.0713999
C	0.4175355	-1.2932860	1.2050001
C	1.6305745	-2.0841380	0.9970761
C	2.0102465	-2.5637850	-0.2343929
C	1.5646665	-1.9090960	-1.3889339
H	0.4531055	-0.2643030	-2.1399319
H	2.1294715	-2.4841380	1.8740181
H	2.8024775	-3.3011000	-0.3035519
H	2.0196135	-2.1213070	-2.3485899
C	-0.1421525	-1.1447490	2.4215601
H	-1.0467595	-0.5479950	2.4931211
B	-0.8381325	0.7231030	0.1128491
O	-1.6745435	1.0849150	1.1370841
O	-0.6642705	1.7415730	-0.7927459
C	-1.2269535	2.9413660	-0.2193869
C	-2.2592445	2.3619860	0.8073391
C	-1.8321575	3.7805850	-1.3343379
H	-2.3335845	4.6626310	-0.9216659
H	-2.5538765	3.2074950	-1.9199569
H	-1.0423775	4.1211250	-2.0099819
C	-0.0726265	3.6928660	0.4460731
H	-0.4049665	4.6446530	0.8713871
H	0.6969905	3.8996240	-0.3033269
H	0.3820065	3.0948050	1.2428881
C	-3.6315225	2.0779410	0.1950951
H	-4.2215945	1.4924570	0.9058031
H	-3.5458975	1.4981830	-0.7289449
H	-4.1705645	3.0047690	-0.0239399
C	-2.4145675	3.1715160	2.0868481
H	-2.7837175	4.1782630	1.8633001

H	-1.4686165	3.2561030	2.6255311
H	-3.1378655	2.6821870	2.7455631
C	3.0540635	0.6811180	-1.9378619
C	4.0374625	-0.5120520	0.5502561
O	2.8602615	0.1511340	-3.0057009
O	4.5640035	-0.9449140	-0.4577719
C	-1.5135885	-1.6066990	-0.4164419
C	-2.1871745	-1.1880030	-1.7350869
C	-1.3157215	-3.1282370	-0.4154389
H	-2.2180795	-1.3856080	0.3998881
C	-3.5377575	-1.8858000	-1.9127049
H	-1.5332705	-1.4586060	-2.5749419
H	-2.3149005	-0.0995240	-1.7882469
C	-2.6583545	-3.8471130	-0.5891339
H	-0.6393095	-3.4153220	-1.2300829
H	-0.8433895	-3.4477080	0.5186111
C	-3.3780925	-3.4074610	-1.8664009
H	-3.9975595	-1.5795120	-2.8596119
H	-4.2185105	-1.5650780	-1.1109499
H	-2.5001825	-4.9318520	-0.5980569
H	-3.2973675	-3.6288330	0.2786291
H	-4.3560125	-3.8969110	-1.9430839
H	-2.7923485	-3.7308780	-2.7384509
C	0.3334045	-1.7096630	3.7288501
H	0.6719065	-0.9085660	4.4000161
H	-0.4907325	-2.2172440	4.2445641
H	1.1494795	-2.4299250	3.6329261
C	2.2043835	0.5646310	-0.6883479
H	1.4658535	1.3607480	-0.6562169
C	2.7732495	0.2130090	0.5328161
H	2.3149285	0.5681820	1.4449051
C	4.1084585	-0.2494020	2.9412631
H	4.7953195	-0.5590880	3.7302481
H	3.1167885	-0.6717610	3.1439661
H	4.0429545	0.8446760	2.9338481
C	4.9377525	1.7409460	-2.8107359
H	5.6483525	2.5011100	-2.4865669
H	4.4290425	2.0548140	-3.7257919
H	5.4481265	0.7910900	-2.9869069
O	4.0121745	1.5977310	-1.7364309
O	4.6564305	-0.7495660	1.7366511

$E_{\text{gas}} = -1490.49565057$

$E_{\text{THF}} = -1490.52465929$

$G_{\text{gas}} = -1489.929936$

$G_{\text{THF}} = -1489.958934$

Imaginary frequency = -432.8188

17f-syn

C	-0.5262238	0.8941260	-1.2605054
C	0.3182852	0.7044020	-0.0233414
C	-0.4809358	1.0192010	1.2475246
C	-1.8934878	1.3988560	1.0453666

C	-2.2733958	2.0575280	-0.1334224
C	-1.6016438	1.7414350	-1.3209554
H	-0.1249338	0.4786910	-2.1797724
H	-2.4785428	1.5980220	1.9356856
H	-3.2101278	2.6039540	-0.1637844
H	-2.0436618	2.0032210	-2.2782134
C	0.0644902	0.9297540	2.4688156
H	1.1011902	0.6065900	2.5301536
B	0.7564902	-0.8247720	0.0014376
O	1.1546532	-1.4932420	1.1308076
O	0.9563972	-1.5565630	-1.1440154
C	1.2587732	-2.9050120	-0.7384334
C	1.8320272	-2.6909170	0.7045896
C	2.2433572	-3.5055240	-1.7321174
H	2.5660192	-4.4994190	-1.4023494
H	3.1257322	-2.8732910	-1.8543594
H	1.7622262	-3.6105050	-2.7089904
C	-0.0557378	-3.6866920	-0.7541084
H	0.1050032	-4.7443150	-0.5211404
H	-0.4950568	-3.6122550	-1.7528424
H	-0.7740558	-3.2656770	-0.0456174
C	3.3297462	-2.3765620	0.7191696
H	3.6094852	-2.0417860	1.7223386
H	3.5729552	-1.5742290	0.0149206
H	3.9302032	-3.2561990	0.4663556
C	1.5216532	-3.8103900	1.6877766
H	1.9501022	-4.7569240	1.3398046
H	0.4453252	-3.9379280	1.8180456
H	1.9577542	-3.5771170	2.6637386
C	1.6086892	1.6031110	-0.1101694
C	2.4904812	1.3085650	-1.3348334
C	1.3068152	3.1064730	-0.0451734
H	2.2038922	1.3508340	0.7802056
C	3.7877542	2.1206420	-1.2908724
H	1.9417582	1.5704120	-2.2504324
H	2.7131622	0.2388450	-1.4084864
C	2.5949042	3.9340200	-0.0048084
H	0.7159992	3.3936630	-0.9257214
H	0.6917332	3.3254360	0.8338896
C	3.5022422	3.6213500	-1.1973974
H	4.3954372	1.9024760	-2.1770674
H	4.3793552	1.8093890	-0.4176084
H	2.3532592	5.0032790	0.0189456
H	3.1351692	3.7133700	0.9271306
H	4.4402892	4.1841230	-1.1233814
H	3.0067602	3.9499410	-2.1220934
C	-0.5798018	1.1749960	3.8006316
H	0.0443692	1.8369030	4.4126276
H	-1.5732508	1.6249510	3.7363626
H	-0.6764968	0.2308760	4.3512496
C	-3.9165818	-0.1919320	-0.0329514
C	-4.1954618	-0.4887620	-1.3634654
C	-4.9399508	0.1537560	0.8480526

C	-5.5071288	-0.4089410	-1.8196784
H	-3.3771048	-0.7799520	-2.0121214
C	-6.2473408	0.2318950	0.3851896
H	-4.7023178	0.3535930	1.8892246
C	-6.5338128	-0.0447310	-0.9515004
H	-5.7292098	-0.6327800	-2.8592004
H	-7.0464408	0.5027020	1.0689686
H	-7.5564248	0.0148920	-1.3119684
N	-2.5753328	-0.3150280	0.5143756
O	-1.7594788	-0.8348270	-0.2904854
$E_{\text{gas}} = -1317.69125077$			
$E_{\text{THF}} = -1317.71504524$			
$G_{\text{gas}} = -1317.1625837$			
$G_{\text{THF}} = -1317.1863782$			
Imaginary frequency = -373.2002			

Li_{(THF)₂}⁺			
Li	-0.1867269	-0.0354896	-0.0480990
C	-0.2444679	-2.4716256	-1.7150400
O	0.4088741	-1.6747596	-0.6899330
C	1.6000471	-2.3545666	-0.2103620
C	1.4865691	-3.7763136	-0.7404700
C	0.7538891	-3.5656196	-2.0685880
H	-1.1657009	-2.8816406	-1.2885080
H	-0.4906999	-1.8121346	-2.5508630
H	2.4743561	-1.8350426	-0.6162190
H	1.6098431	-2.2885666	0.8804180
H	2.4639201	-4.2472716	-0.8614560
H	0.8891261	-4.3928376	-0.0615910
H	1.4461091	-3.2192216	-2.8422430
H	0.2572081	-4.4676396	-2.4309700
C	-0.1334779	2.8938824	0.0363980
O	-0.6038709	1.6485524	0.6179920
C	-1.3938539	1.9193424	1.8083060
C	-1.6214899	3.4252774	1.8046930
C	-0.3557619	3.9427064	1.1151980
H	0.9144921	2.7610524	-0.2438060
H	-0.7283099	3.0986424	-0.8598070
H	-2.3149589	1.3348684	1.7447560
H	-0.8137469	1.5955194	2.6785870
H	-2.5110969	3.6786884	1.2200350
H	-1.7508079	3.8205054	2.8139230
H	-0.4760449	4.9425984	0.6940440
H	0.4865801	3.9610934	1.8136040
$E_{\text{gas}} = -472.321628425$			
$E_{\text{THF}} = -472.395718419$			
$E_{\text{CHCl}_3} = -472.392397681$			
$G_{\text{gas}} = -472.123107$			
$G_{\text{THF}} = -472.197197$			
$G_{\text{CHCl}_3} = -472.193877$			

LiB(CH₃)₄

Li	1.9354537	0.0601456	-0.0484818
C	-1.6903893	-0.0598354	0.0438722
H	-2.0611203	-0.5390174	0.9608622
H	-2.1398263	0.9422326	0.0029392
H	-2.1023373	-0.6287234	-0.8013938
C	0.5012057	-1.5835714	0.0671962
H	0.1279217	-2.0589384	0.9825262
H	0.0945357	-2.1434784	-0.7837498
H	1.5887187	-1.8495114	0.0600172
C	0.3834167	0.7462306	-1.4351688
H	-0.0053483	0.1649766	-2.2803888
H	-0.0792673	1.7397716	-1.4782218
H	1.4486687	0.9431136	-1.7165748
C	0.4501737	0.8862416	1.3335742
H	1.5279487	1.0990046	1.5482812
H	-0.0043033	1.8836246	1.2927742
H	0.0945917	0.3989526	2.2497922
B	-0.0700423	-0.0012174	0.0021452

$E_{\text{gas}} = -192.083850025$

$E_{\text{THF}} = -192.099165600$

$E_{\text{CHCl}_3} = -192.098555615$

$G_{\text{gas}} = -191.959744$

$G_{\text{THF}} = -191.975059$

$G_{\text{CHCl}_3} = -191.974496$

Li⁺

Li	0.0000000	0.0000000	0.0000000
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$E_{\text{gas}} = -7.29270972417$

$E_{\text{THF}} = -7.41714868764$

$E_{\text{CHCl}_3} = -7.40627609425$

$G_{\text{gas}} = -7.305458$

$G_{\text{THF}} = -7.429897$

$G_{\text{CHCl}_3} = -7.419024$