

## Supplementary Material

### **The mechanism of cleavage of Evans chiral auxiliaries by LiOOH: origins of the different regioselectivities obtained with LiOH, LiOOH, LiOBn and LiSBn**

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## Computed Geometries and Energies

The Cartesian coordinates of optimised geometries are listed below, along with the following energies (all in Hartree):

$E_{\text{B3LYP-D3}} = \text{B3LYP-D3/6-31+G(d)}$  electronic potential energy plus solvation correction in SMD water

$G_{\text{B3LYP-D3}} = \text{B3LYP-D3/6-31+G(d)}$  Gibbs free energy (quasiharmonically corrected) in SMD water at 298.15 K and 1 mol L<sup>-1</sup>

$E_{\text{M06-2X-D3}} = \text{M06-2X-D3/6-311+G(d,p)}$  single-point electronic potential energy in SMD water, calculated at the B3LYP-D3 optimised geometry

$G_{\text{tot}} = \text{total M06-2X-D3/6-311+G(d,p)//B3LYP-D3/6-31+G(d)}$  Gibbs free energy in SMD water at 298.15 K and 1 mol L<sup>-1</sup>

## Reactions involving OH<sup>-</sup>

5

N	0.765662	-0.370112	-0.098030
C	2.215214	-0.678923	0.073667
C	2.277072	-2.034931	-0.635056
O	0.918072	-2.563118	-0.508331
C	0.061985	-1.556731	-0.298398
C	0.166631	0.880532	0.010326
H	2.818037	0.052998	-0.462018
H	2.493489	-1.948054	-1.702051
O	-1.150137	-1.729975	-0.294477
H	2.949870	-2.745218	-0.156512
O	-1.064049	0.994750	0.002996
C	1.071988	2.096064	0.047573
C	1.412467	2.479431	-1.411691
C	0.397040	3.255762	0.787225
H	1.090874	4.101834	0.835102
H	2.000592	1.845308	0.565898
C	2.591745	-0.755102	1.550645
H	2.013662	-1.540213	2.051735
H	3.657377	-0.992501	1.637656
H	0.499903	2.734781	-1.962398
H	2.070750	3.354660	-1.406012
H	0.127202	2.972470	1.810744
H	-0.509136	3.583944	0.267886
H	1.924023	1.668126	-1.940690
H	2.402947	0.196548	2.056810
Li	-2.452796	-0.334330	0.020478
O	-3.332094	-0.598595	1.723813
H	-4.034863	0.041030	1.931507
O	-3.821110	-0.100492	-1.321725
H	-4.700542	0.125571	-0.972799
H	-3.635487	0.582027	-1.989570
H	-2.740252	-0.576712	2.495539

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -753.585708$

$G_{\text{B3LYP-D3}} = -753.366448$

$E_{M06-2X-D3} = -753.455738$

$G_{tot} = -753.236478$

### OH<sup>-</sup>

O 0.000000 0.000000 0.107899  
H 0.000000 0.000000 -0.863196

0 imaginary frequencies

$E_{B3LYP-D3} = -75.948934$

$G_{B3LYP-D3} = -75.953664$

$E_{M06-2X-D3} = -75.939503$

$G_{tot} = -75.944233$

### TSA

N -0.724078 -0.287489 -0.208244  
C -2.136907 -0.741801 -0.148647  
C -1.932695 -2.211786 0.238425  
O -0.638516 -2.543151 -0.321815  
C 0.149654 -1.426608 -0.283655  
C -0.266943 0.987403 -0.065109  
H -2.669252 -0.212858 0.642808  
H -1.892679 -2.356685 1.320603  
O 1.256238 -1.435189 -0.848471  
H -2.666223 -2.879562 -0.213266  
O 0.954877 1.243406 -0.084662  
C -1.271912 2.099183 0.189953  
C -1.391792 2.282496 1.718481  
C -0.837313 3.397441 -0.500230  
H -1.594901 4.170236 -0.329002  
H -2.250526 1.812265 -0.199555  
C -2.838086 -0.585861 -1.497619  
H -2.331618 -1.186188 -2.262041  
H -3.873885 -0.932467 -1.409586  
H -0.426599 2.576187 2.147048  
H -2.120720 3.071534 1.934205  
H -0.729439 3.256050 -1.581954  
H 0.116755 3.758198 -0.102268  
O 0.612117 -1.471355 1.695389  
H -1.724637 1.362214 2.211675  
H -2.847814 0.457669 -1.826625  
Li 2.422725 0.027033 -0.357139  
O 3.768827 0.663898 -1.597166  
H 4.677507 0.662858 -1.249993  
O 3.012943 -0.559771 1.408503  
H 3.138769 0.181794 2.023226  
H 2.073165 -0.935555 1.614076  
H 3.627281 1.571973 -1.916653  
H 0.719270 -2.431847 1.802618

1 imaginary frequency ( $312.9i \text{ cm}^{-1}$ )

$E_{B3LYP-D3} = -829.544746$

$G_{B3LYP-D3} = -829.314200$

$E_{M06-2X-D3} = -829.408664$

$G_{tot} = -829.178119$

### TSB

N -0.610797 -0.485250 -0.190313  
C -1.892795 -1.029630 0.333906  
C -1.492432 -2.488255 0.591776  
O -0.349734 -2.705447 -0.289471  
C 0.217373 -1.509213 -0.565051  
C -0.150201 0.865961 0.026463

H	-2.127157	-0.528289	1.272635
H	-1.152449	-2.659455	1.616393
O	1.326598	-1.455898	-1.102505
H	-2.263208	-3.207432	0.316579
O	1.008838	1.166444	-0.350172
C	-1.243409	1.935481	-0.004115
C	-0.810236	3.232494	0.688393
C	-1.563299	2.222054	-1.489147
H	-2.427334	2.892750	-1.555289
H	-2.141201	1.558165	0.490447
C	-3.047966	-0.915294	-0.659087
H	-2.789125	-1.393926	-1.610779
H	-3.922244	-1.426551	-0.239956
H	0.143482	3.593036	0.287717
H	-1.564942	4.007445	0.511878
H	-1.794915	1.312790	-2.052418
H	-0.710045	2.712482	-1.972060
O	0.046851	0.574357	2.043208
H	-0.709104	3.109261	1.770904
H	-3.324068	0.123759	-0.851100
Li	2.463760	-0.068436	-0.246467
O	4.172659	0.256417	-1.071723
H	4.788050	0.798904	-0.548905
O	2.370419	-0.544847	1.653154
H	1.450770	-0.135606	1.865930
H	2.252276	-1.503989	1.756105
H	4.141009	0.689220	-1.942470
H	0.327263	1.449706	2.357234

1 imaginary frequency ( $238.1i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -829.542108$

$G_{\text{B3LYP-D3}} = -829.310906$

$E_{\text{M06-2X-D3}} = -829.406275$

$G_{\text{tot}} = -829.175074$

## TSC

(C–N bond cleavage step after an initial proton transfer from OH to O<sup>-</sup> in **6**)

N	0.671524	0.432834	-0.351500
C	1.822096	1.224329	0.061986
C	1.205043	2.546617	0.552623
O	0.000812	2.213381	1.282538
C	-0.912266	1.512012	0.542153
C	0.636320	-0.883130	-0.304876
H	2.341680	0.766492	0.915334
H	0.955116	3.208373	-0.283198
H	1.848670	3.073820	1.257845
O	-0.468985	-1.513964	-0.514808
C	1.860819	-1.739635	0.036659
C	1.729994	-2.220861	1.494352
C	2.011045	-2.920934	-0.931509
H	2.915017	-3.492284	-0.687293
H	2.764181	-1.128684	-0.038124
C	2.829047	1.499675	-1.058303
H	2.326756	1.956807	-1.919604
H	3.613007	2.185308	-0.711165
H	0.839643	-2.849310	1.617000
H	2.608450	-2.813429	1.778094
H	2.096538	-2.576151	-1.969584
H	1.152238	-3.598183	-0.866674
O	-1.647330	0.676934	1.110411
H	1.649961	-1.375307	2.188540
H	3.309013	0.573951	-1.392739

Li	-2.156406	-0.797008	-0.077297
O	-2.921768	0.221558	-1.621520
H	-2.633073	-0.040391	-2.513306
O	-3.406501	-2.083714	0.683195
H	-3.929374	-1.742916	1.429493
H	-2.950748	-2.865766	1.040020
H	-3.874839	0.400764	-1.700134
O	-1.351891	2.225769	-0.537744
H	-1.990976	1.649941	-1.027209

1 imaginary frequency (196.0i cm<sup>-1</sup>)

E<sub>B3LYP-D3</sub> = -829.540754

G<sub>B3LYP-D3</sub> = -829.310288

E<sub>M06-2X-D3</sub> = -829.409486

G<sub>tot</sub> = -829.179020

## TSD

N	0.768537	0.063231	-0.284024
C	2.102615	0.535666	0.230856
C	3.149714	-0.562877	-0.029562
O	2.803131	-1.772052	0.570818
C	0.518633	-1.348454	-0.438500
C	-0.330691	0.847648	-0.464545
H	2.375926	1.420129	-0.350880
H	3.270507	-0.654701	-1.129016
O	-0.227630	-1.983307	0.301317
H	4.108259	-0.146894	0.344835
O	-1.437490	0.323329	-0.744848
C	-0.230973	2.360684	-0.377578
C	-0.560599	2.955532	-1.759568
C	-1.199900	2.874303	0.702073
H	-1.123732	3.965210	0.769105
H	0.781689	2.662395	-0.109471
C	1.993051	0.878421	1.717600
H	1.720470	-0.010009	2.295420
H	2.963394	1.242664	2.075400
H	-1.583518	2.704244	-2.059715
H	-0.471692	4.046597	-1.714376
H	-0.962483	2.454101	1.686724
H	-2.234477	2.614543	0.453510
O	0.960932	-1.794969	-1.614600
H	0.128946	2.585887	-2.527509
H	1.246737	1.655437	1.907388
Li	-2.077738	-1.180989	0.327487
O	-2.566815	-0.416235	2.040582
H	-3.519235	-0.272661	2.176434
O	-3.300432	-2.471597	-0.404465
H	-4.060326	-2.117828	-0.898646
H	-2.874407	-3.096624	-1.016838
H	-2.170131	0.468913	2.124933
H	0.752858	-2.747941	-1.696667

1 imaginary frequency (56.0i cm<sup>-1</sup>)

E<sub>B3LYP-D3</sub> = -829.519500

G<sub>B3LYP-D3</sub> = -829.289519

E<sub>M06-2X-D3</sub> = -829.384627

G<sub>tot</sub> = -829.154647

## TSE

N	-0.818488	-0.571084	-0.251007
C	-2.195685	-0.869241	0.187962
C	-2.200475	-2.408532	0.297477
O	-0.799709	-2.775974	0.313100

C	-0.075501	-1.659943	-0.078016
C	0.052544	1.030276	0.404085
H	-2.346315	-0.422700	1.180671
H	-2.668177	-2.785615	1.208906
O	1.163074	-1.809790	-0.208580
H	-2.662475	-2.877819	-0.578267
O	1.206933	1.057398	-0.125788
C	-0.970563	2.110509	0.046375
C	-0.548799	3.433025	0.716708
C	-1.090927	2.296381	-1.467300
H	-1.874540	3.029390	-1.692052
H	-1.937187	1.816460	0.465107
C	-3.289279	-0.379295	-0.758134
H	-3.113531	-0.750963	-1.774663
H	-4.260629	-0.760520	-0.417470
H	0.437817	3.753852	0.361053
H	-1.270365	4.219135	0.464697
H	-1.342391	1.360644	-1.973472
H	-0.148825	2.669333	-1.886656
O	-0.014942	0.753974	1.778428
H	-0.510780	3.343239	1.807161
H	-3.352229	0.711254	-0.791645
Li	2.412563	-0.371814	-0.291774
O	3.563282	-0.437153	-1.873850
H	4.321016	0.171428	-1.831018
O	3.643124	-0.345521	1.257799
H	3.153535	-0.049716	2.044988
H	4.003995	-1.214176	1.505275
H	3.103035	-0.199292	-2.697486
H	0.777783	0.236536	2.013440

1 imaginary frequency ( $246.5i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -829.545154$

$G_{\text{B3LYP-D3}} = -829.314861$

$E_{\text{M06-2X-D3}} = -829.415038$

$G_{\text{tot}} = -829.184745$

## 6

N	-0.735027	-0.326849	0.081422
C	-2.142486	-0.777728	-0.000850
C	-1.962086	-2.277835	0.258567
O	-0.692014	-2.578810	-0.340986
C	0.208979	-1.508278	-0.030778
C	-0.292341	0.937457	0.186793
H	-2.732975	-0.320815	0.796581
H	-1.938997	-2.504172	1.331017
O	1.183816	-1.416004	-0.884705
H	-2.721631	-2.888112	-0.232941
O	0.939029	1.205341	0.193802
C	-1.286307	2.085142	0.318719
C	-1.044418	2.810485	1.654122
C	-1.128508	3.039485	-0.877251
H	-1.854735	3.856231	-0.795410
H	-2.307965	1.702138	0.322513
C	-2.766176	-0.500379	-1.370290
H	-2.214400	-1.029536	-2.155353
H	-3.804638	-0.851207	-1.375546
H	-0.039060	3.244176	1.688261
H	-1.772941	3.621296	1.768306
H	-1.300429	2.520989	-1.827742
H	-0.122896	3.474168	-0.898083
O	0.661215	-1.715681	1.353887

H	-1.155831	2.127228	2.504643
H	-2.762085	0.567801	-1.606925
Li	2.325468	0.032843	-0.453540
O	3.604254	0.761755	-1.722408
H	4.410920	1.110494	-1.305396
O	3.183332	-0.463933	1.303507
H	3.260622	0.330161	1.858936
H	2.320948	-0.867894	1.557830
H	3.264303	1.500165	-2.256790
H	1.083564	-2.595129	1.357790

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -829.558136$

$G_{\text{B3LYP-D3}} = -829.324943$

$E_{\text{M06-2X-D3}} = -829.429626$

$G_{\text{tot}} = -829.196434$

7

N	-0.413695	0.198367	-0.206079
C	-0.362748	1.656817	-0.176862
C	0.936767	2.143312	-0.821359
O	2.098877	1.711000	-0.036022
C	2.616474	0.500248	-0.209823
C	-1.547180	-0.462491	-0.166667
H	-1.147393	2.111158	-0.802193
H	1.040442	1.791406	-1.848007
O	3.227324	-0.056957	0.702042
H	0.996459	3.232500	-0.798041
O	-1.493652	-1.768207	-0.104927
C	-2.945077	0.159518	-0.182309
C	-3.714128	-0.292995	-1.435374
C	-3.708041	-0.210078	1.100882
H	-4.692689	0.273686	1.106777
H	-2.857678	1.248976	-0.217057
C	-0.507781	2.194683	1.255466
H	0.260791	1.762217	1.906509
H	-0.411610	3.287598	1.280341
H	-3.859921	-1.379342	-1.435691
H	-4.702189	0.183006	-1.464285
H	-3.163951	0.114544	1.996355
H	-3.860173	-1.293487	1.167560
O	2.473869	-0.011515	-1.433376
H	-3.177904	-0.019402	-2.352678
H	-1.487278	1.923633	1.663240
Li	0.394915	-1.653848	0.262504
O	1.234915	-1.624086	2.049464
H	0.703519	-1.070185	2.646798
O	1.818089	-2.554942	-0.803399
H	2.455178	-3.098515	-0.307428
H	1.543451	-3.102980	-1.559593
H	2.034459	-1.088933	1.867067
H	2.552504	-0.999337	-1.368609

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -829.547780$

$G_{\text{B3LYP-D3}} = -829.316374$

$E_{\text{M06-2X-D3}} = -829.415469$

$G_{\text{tot}} = -829.184063$

9

N	0.590139	-0.306583	0.145655
C	2.089358	-0.084019	0.198384
C	2.891289	-0.974826	-0.801115

O	4.083772	-0.342009	-1.170280
C	0.039072	-1.556858	0.391721
C	-0.257523	0.763453	-0.190963
H	2.224593	0.916698	-0.204545
H	3.077753	-1.956441	-0.331495
O	-1.165145	-1.823794	0.423272
H	2.220954	-1.166330	-1.667391
O	-1.369652	0.571786	-0.692216
C	0.187137	2.189568	0.096736
C	0.538755	2.905508	-1.221470
C	-0.955786	2.911290	0.835430
H	-0.625774	3.921754	1.100251
H	1.058882	2.186391	0.753014
C	2.614563	-0.120306	1.629888
H	2.464976	-1.102318	2.088642
H	3.689153	0.091569	1.613805
H	-0.330449	2.925601	-1.888492
H	0.833463	3.938083	-1.005373
H	-1.227527	2.385662	1.758791
H	-1.846743	2.991642	0.204564
O	0.963155	-2.483963	0.652061
H	1.365974	2.413097	-1.744860
H	2.126149	0.637231	2.253525
Li	-2.645008	-0.778133	-0.192498
O	-3.608240	0.166350	1.217551
H	-4.560998	0.321492	1.100900
O	-3.800592	-1.662802	-1.452356
H	-4.307557	-1.073345	-2.037216
H	-3.353660	-2.283716	-2.053564
H	-3.220230	1.053780	1.318312
H	0.507511	-3.327771	0.843124

0 imaginary frequencies

$E_{B3LYP-D3} = -829.524586$

$G_{B3LYP-D3} = -829.294767$

$E_{M06-2X-D3} = -829.390004$

$G_{tot} = -829.160185$

## 10

N	-0.619011	-0.498013	-0.108994
C	-1.913189	-1.049650	0.373295
C	-1.540277	-2.524282	0.571056
O	-0.404560	-2.717921	-0.320080
C	0.188857	-1.501884	-0.515400
C	-0.113693	0.897746	0.261165
H	-2.166417	-0.584467	1.327456
H	-1.205422	-2.744252	1.589108
O	1.318137	-1.464505	-1.027325
H	-2.324361	-3.218736	0.269111
O	1.040047	1.199145	-0.296035
C	-1.242254	1.933812	-0.004865
C	-0.915845	3.290396	0.638252
C	-1.460290	2.112021	-1.514068
H	-2.350018	2.726274	-1.697603
H	-2.165412	1.565275	0.454523
C	-3.054983	-0.883471	-0.631126
H	-2.788263	-1.334418	-1.594316
H	-3.943496	-1.395895	-0.243526
H	0.048760	3.673006	0.284355
H	-1.686262	4.021994	0.367088
H	-1.597436	1.156315	-2.029621
H	-0.600166	2.618037	-1.968058



O	0.030893	0.720093	1.747617
H	-0.888396	3.240231	1.733100
H	-3.314073	0.164427	-0.795544
Li	2.431155	-0.035318	-0.261155
O	4.167690	0.218116	-1.082410
H	4.787273	0.757742	-0.561643
O	2.483366	-0.598523	1.680697
H	1.593175	-0.203536	1.860205
H	2.343739	-1.559410	1.732443
H	4.145123	0.645158	-1.956248
H	0.376715	1.564933	2.086018

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -829.552010$

$G_{\text{B3LYP-D3}} = -829.318055$

$E_{\text{M06-2X-D3}} = -829.424194$

$G_{\text{tot}} = -829.190239$

## 11

N	3.031788	-0.223271	1.092956
C	3.447254	1.047675	0.474853
C	2.554762	1.176859	-0.774869
O	1.458095	0.270021	-0.498962
C	1.907996	-0.590111	0.558575
C	-1.941747	0.696096	0.218533
H	3.219268	1.867795	1.171257
H	2.146167	2.176473	-0.936043
O	1.136443	-1.564039	0.809237
H	3.059835	0.827851	-1.683500
O	-1.831142	-0.531679	0.205898
C	-3.254706	1.422569	0.401040
C	-3.794435	1.802582	-0.995808
C	-4.262514	0.578768	1.184994
H	-5.182145	1.154549	1.336595
H	-3.036139	2.346912	0.947755
C	4.932821	1.102069	0.142885
H	5.206998	0.289616	-0.541963
H	5.182652	2.056810	-0.337626
H	-3.999203	0.902510	-1.587746
H	-4.730833	2.359786	-0.882706
H	-3.868721	0.294718	2.167466
H	-4.518147	-0.336144	0.639029
O	-0.905289	1.516608	0.030986
H	-3.083918	2.428827	-1.545663
H	5.539652	1.010134	1.051171
Li	-0.482548	-1.892848	-0.146952
O	-1.201719	-3.671621	0.158297
H	-2.165212	-3.742675	0.043448
O	-0.041261	-1.496379	-2.068963
H	0.613611	-0.806516	-1.824851
H	0.480180	-2.198996	-2.492395
H	-1.036474	-4.005103	1.057272
H	-0.060050	1.012539	-0.144489

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -829.569905$

$G_{\text{B3LYP-D3}} = -829.340872$

$E_{\text{M06-2X-D3}} = -829.432589$

$G_{\text{tot}} = -829.203556$

## Reactions involving OOH<sup>-</sup>

### OOH<sup>-</sup>

O	0.055915	-0.694845	0.000000
H	-0.894647	-0.900550	0.000000
O	0.055915	0.807414	0.000000

0 imaginary frequencies

E<sub>B3LYP-D3</sub> = -151.089225

G<sub>B3LYP-D3</sub> = -151.094764

E<sub>M06-2X-D3</sub> = -151.069651

G<sub>tot</sub> = -151.075189

### TSF

N	0.842980	-0.320494	0.296856
C	2.156615	-1.017703	0.239396
C	1.684574	-2.459966	0.023490
O	0.365416	-2.493866	0.632375
C	-0.180830	-1.260811	0.562666
C	0.600442	1.001222	0.024391
H	2.725370	-0.675191	-0.625144
H	1.575415	-2.711185	-1.033729
O	-1.299496	-1.036409	1.026570
H	2.301571	-3.196507	0.537368
O	-0.548045	1.474475	0.103199
C	1.756585	1.867395	-0.444592
C	1.795006	1.807314	-1.988215
C	1.598426	3.307547	0.056521
H	2.463906	3.897846	-0.263900
H	2.697573	1.469341	-0.059584
C	2.941904	-0.838329	1.536783
H	2.379074	-1.247429	2.383653
H	3.895530	-1.372004	1.458480
H	0.864395	2.203841	-2.410132
H	2.629119	2.416627	-2.353158
H	1.542841	3.344704	1.150574
H	0.695660	3.773379	-0.351748
O	-0.684082	-1.326427	-1.678591
O	-2.056971	-1.874442	-1.769655
H	-2.593710	-1.114517	-1.459970
H	1.930858	0.782802	-2.351495
H	3.149058	0.218160	1.733254
Li	-2.171272	0.629819	0.651119
O	-3.122231	1.352583	2.177095
H	-3.731591	2.081988	1.969956
O	-3.384999	0.504743	-0.863046
H	-4.345690	0.411246	-0.744879
H	-3.273655	1.134101	-1.596734
H	-2.565838	1.691533	2.899621

1 imaginary frequency (125.9i cm<sup>-1</sup>)

E<sub>B3LYP-D3</sub> = -904.683360

G<sub>B3LYP-D3</sub> = -904.450979

E<sub>M06-2X-D3</sub> = -904.536891

G<sub>tot</sub> = -904.304511

### TSG

N	0.849465	-0.473458	0.250172
C	2.214150	-0.742797	-0.284243
C	2.068440	-2.209685	-0.717365
O	0.918679	-2.701092	0.033916
C	0.168328	-1.655999	0.427865

C	0.197210	0.783806	0.183678
H	2.380197	-0.111819	-1.157572
H	1.833695	-2.317022	-1.778739
O	-0.955845	-1.832812	0.897367
H	2.924674	-2.827085	-0.447434
O	-1.010982	0.873835	0.459744
C	1.078075	2.023490	0.215357
C	0.419437	3.214243	-0.488147
C	1.333997	2.359266	1.704526
H	2.037879	3.196252	1.772083
H	2.034040	1.816542	-0.269630
C	3.313158	-0.548109	0.756215
H	3.120893	-1.166842	1.640415
H	4.269810	-0.854739	0.318245
H	-0.555557	3.444578	-0.045179
H	1.059127	4.097164	-0.376686
H	1.754208	1.513367	2.257818
H	0.397638	2.655604	2.191390
O	0.045873	0.480271	-2.138652
O	-1.293615	1.003824	-2.482347
H	-1.884149	0.415411	-1.966138
H	0.280517	3.017906	-1.554080
H	3.401912	0.495075	1.067684
Li	-2.321826	-0.475065	0.686080
O	-3.659872	-0.256253	2.055731
H	-4.472956	0.190008	1.761679
O	-3.060078	-0.826625	-1.080974
H	-2.840199	-1.689758	-1.473243
H	-3.984809	-0.658590	-1.330244
H	-3.367755	0.248862	2.834577

1 imaginary frequency ( $114.2i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -904.680628$

$G_{\text{B3LYP-D3}} = -904.449014$

$E_{\text{M06-2X-D3}} = -904.534208$

$G_{\text{tot}} = -904.302594$

## TSH

N	-0.500430	0.618239	-0.117905
C	-0.957206	1.992412	-0.040647
C	0.323063	2.825492	-0.234850
O	1.382128	2.189249	0.550207
C	1.746571	0.951682	0.170200
C	-1.257877	-0.440721	-0.225665
H	-1.640613	2.264809	-0.859023
H	0.629766	2.873682	-1.282265
O	2.137345	0.094392	0.957435
H	0.242420	3.833471	0.172541
O	-0.724695	-1.623389	-0.137951
C	-2.767992	-0.388267	-0.478629
C	-3.097716	-1.058039	-1.824083
C	-3.533413	-1.057718	0.674470
H	-4.614708	-0.984315	0.504007
H	-3.084910	0.657424	-0.538134
C	-1.619836	2.324054	1.305292
H	-0.922653	2.135913	2.130634
H	-1.920188	3.378882	1.337893
H	-2.830232	-2.120886	-1.809638
H	-4.172389	-0.980372	-2.030665
H	-3.306998	-0.580594	1.635741
H	-3.272518	-2.119764	0.750781
O	2.062737	0.924806	-1.186608

O	3.030658	-0.100842	-1.497631
H	2.537900	-0.959472	-1.371324
H	-2.557008	-0.580095	-2.650535
H	-2.509967	1.707691	1.465661
Li	1.016043	-1.660623	0.637479
O	1.229402	-2.453352	2.400724
H	0.455595	-2.942272	2.729666
O	1.985244	-2.529631	-0.852341
H	2.768009	-3.104100	-0.789129
H	1.405351	-2.941283	-1.517040
H	1.411911	-1.787761	3.086512

1 imaginary frequency ( $112.6i$  cm<sup>-1</sup>)

E<sub>B3LYP-D3</sub> = -904.663191

G<sub>B3LYP-D3</sub> = -904.430523

E<sub>M06-2X-D3</sub> = -904.520037

G<sub>tot</sub> = -904.287370

## TSI

N	1.046542	-0.572056	0.330837
C	2.389289	-0.695178	-0.267620
C	2.541418	-2.218454	-0.464035
O	1.185027	-2.725606	-0.397819
C	0.402376	-1.714065	0.148926
C	-0.196583	1.044973	-0.095799
H	2.386432	-0.193008	-1.245555
H	2.971386	-2.501311	-1.426686
O	-0.798025	-1.998068	0.391470
H	3.114780	-2.678307	0.349305
O	-1.224261	0.910349	0.587773
C	0.792448	2.176617	0.123567
C	0.193216	3.455733	-0.498315
C	1.100978	2.377524	1.607689
H	1.855826	3.163181	1.727296
H	1.707481	1.935572	-0.423696
C	3.513297	-0.116356	0.586421
H	3.497244	-0.554604	1.591688
H	4.482494	-0.347160	0.125751
H	-0.744359	3.731180	-0.001255
H	0.901215	4.283236	-0.374168
H	1.483163	1.460417	2.064510
H	0.200781	2.685394	2.152640
O	-0.255267	0.654334	-1.486103
O	-1.536982	1.053221	-2.055248
H	-2.136586	0.314216	-1.773567
H	-0.003629	3.332560	-1.568215
H	3.435791	0.970614	0.679583
Li	-2.203016	-0.745618	0.626191
O	-3.389559	-0.915289	2.152205
H	-4.310127	-0.656101	1.974122
O	-3.189868	-0.939297	-1.074964
H	-3.047553	-1.778632	-1.546928
H	-4.127157	-0.717879	-1.212150
H	-3.131087	-0.390039	2.929375

1 imaginary frequency ( $229.4i$  cm<sup>-1</sup>)

E<sub>B3LYP-D3</sub> = -904.676808

G<sub>B3LYP-D3</sub> = -904.445001

E<sub>M06-2X-D3</sub> = -904.534027

G<sub>tot</sub> = -904.302221

## TSJ

N	0.656382	-0.491353	0.379467
C	1.997010	-1.078579	0.097983
C	1.659032	-2.564702	0.151972
O	0.299726	-2.652507	-0.331304
C	-0.304387	-1.395240	-0.221659
C	0.326680	0.857324	-0.014004
H	2.310153	-0.815589	-0.919686
H	2.296767	-3.169424	-0.494763
O	-1.530380	-1.518066	0.456731
H	1.693355	-2.950878	1.177419
O	-0.813282	1.280609	0.355754
C	1.451668	1.873512	-0.188586
C	1.055010	2.964510	-1.193090
C	1.768891	2.505176	1.181847
H	1.983356	1.755215	1.949790
H	2.341564	1.369841	-0.572272
C	3.091417	-0.731154	1.100510
H	3.937870	-1.410313	0.939634
H	3.463851	0.288284	0.984779
H	0.138442	3.475714	-0.878358
H	1.855390	3.711251	-1.255871
H	0.920267	3.107887	1.525676
H	2.641704	3.162324	1.093419
O	-0.701820	-0.917258	-1.514807
O	0.072470	0.276080	-1.846253
H	-1.378937	-2.007608	1.286330
H	0.894370	2.552481	-2.194395
H	2.736365	-0.864377	2.128268
Li	-2.416039	0.314924	0.552793
O	-3.273968	0.172902	-1.224874
H	-2.455324	-0.210084	-1.611866
O	-3.571941	0.637274	2.058263
H	-4.323945	0.027373	2.152033
H	-3.387511	1.029970	-1.668986
H	-3.132667	0.625290	2.926298

l imaginary frequency (177.9i cm<sup>-1</sup>)

E<sub>B3LYP-D3</sub> = -904.659124

G<sub>B3LYP-D3</sub> = -904.422553

E<sub>M06-2X-D3</sub> = -904.523096

G<sub>tot</sub> = -904.286525

## TSK

N	1.033038	-0.274802	0.385966
C	2.248451	-0.253673	-0.493702
C	2.279054	-1.673058	-1.091468
O	1.328811	-2.425469	-0.273279
C	0.553113	-1.533839	0.339850
C	-0.085503	0.796250	0.154823
H	2.090410	0.464871	-1.296957
H	1.929169	-1.714576	-2.124533
O	-0.295810	-2.016740	1.234961
H	3.243721	-2.171086	-0.991799
O	-1.072019	0.644652	1.007023
C	0.519506	2.216772	0.073737
C	-0.513333	3.196236	-0.506821
C	0.978441	2.682176	1.461226
H	1.685196	1.981573	1.917356
H	1.385120	2.205306	-0.595725
C	3.502498	0.103422	0.293316
H	4.371321	0.080936	-0.375162

H	3.422014	1.107678	0.719698
H	-1.427748	3.204058	0.098246
H	-0.100383	4.212175	-0.508323
H	0.122520	2.790281	2.137302
H	1.473319	3.657523	1.381395
O	-0.870924	-0.974950	-1.166685
O	-0.474315	0.428827	-1.237357
H	-0.519846	-2.943636	1.018622
H	-0.786357	2.941842	-1.536286
H	3.670692	-0.613726	1.105340
Li	-2.301343	-0.510888	0.103971
O	-3.255571	0.797143	-1.162403
H	-2.336947	1.022472	-1.427337
O	-3.461872	-1.802071	0.974332
H	-4.127253	-2.218421	0.399951
H	-3.558963	1.575864	-0.665568
H	-2.942980	-2.543702	1.331599

1 imaginary frequency ( $173.9i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -904.641814$

$G_{\text{B3LYP-D3}} = -904.406369$

$E_{\text{M06-2X-D3}} = -904.503765$

$G_{\text{tot}} = -904.268320$

## 12

N	-0.993493	-0.077578	-0.133599
C	-2.379734	0.000418	0.373586
C	-2.494433	-1.384714	1.014144
O	-1.707336	-2.227402	0.150428
C	-0.575841	-1.509011	-0.317386
C	-0.151485	0.951424	-0.341228
H	-2.458139	0.778349	1.135308
H	-2.082798	-1.397544	2.030216
O	-0.132344	-1.882870	-1.464168
H	-3.514500	-1.772133	1.020005
O	1.042167	0.758726	-0.684330
C	-0.641485	2.373284	-0.099524
C	-0.212744	2.792351	1.322059
C	-0.082233	3.330954	-1.158936
H	-0.469603	4.340092	-0.978493
H	-1.731618	2.402999	-0.153159
C	-3.398926	0.219158	-0.745033
H	-3.364276	-0.607893	-1.462923
H	-4.406901	0.270332	-0.317804
H	0.880310	2.824156	1.400694
H	-0.599664	3.793493	1.543092
H	-0.379546	3.025142	-2.168959
H	1.011287	3.371080	-1.118542
O	0.487431	-1.746621	0.783810
O	1.730183	-2.144201	0.128041
H	1.356106	-2.289115	-0.798278
H	-0.596893	2.100305	2.080746
H	-3.202010	1.152251	-1.282617
Li	2.432023	-0.290700	0.070521
O	4.048390	-0.375522	-1.013870
H	4.280540	0.460112	-1.454911
O	2.747064	0.449784	1.851286
H	1.933499	0.892640	2.149865
H	2.937396	-0.207852	2.542045
H	3.962030	-1.019593	-1.738311

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -904.687925$

$G_{B3LYP-D3} = -904.453945$   
 $E_{M06-2X-D3} = -904.548052$   
 $G_{tot} = -904.314072$

### 13

N	-0.663349	0.220600	-0.101369
C	-0.690890	1.654375	-0.373075
C	0.648700	2.091567	-0.959374
O	1.720415	1.916523	0.040191
C	2.507825	0.858352	0.079955
C	-1.767237	-0.488625	-0.020209
H	-1.410972	1.908526	-1.167327
H	0.896477	1.544102	-1.867559
O	3.150613	0.552184	1.068985
H	0.656395	3.163349	-1.162656
O	-1.662680	-1.753466	0.287293
C	-3.184447	0.033634	-0.266788
C	-3.821587	-0.706373	-1.455519
C	-4.037832	-0.119503	1.003468
H	-5.041299	0.290918	0.835569
H	-3.143665	1.097021	-0.517728
C	-1.039026	2.475810	0.878596
H	-0.326212	2.269679	1.684959
H	-1.016661	3.551208	0.661079
H	-3.922497	-1.776998	-1.243900
H	-4.821892	-0.303673	-1.657714
H	-3.590379	0.412135	1.852179
H	-4.143077	-1.175270	1.278669
O	2.546041	0.196465	-1.115053
O	3.413113	-0.952129	-1.055872
H	2.734388	-1.676642	-0.918444
H	-3.218934	-0.592726	-2.365313
H	-2.040146	2.217544	1.238090
Li	0.247145	-1.532377	0.489146
O	1.312297	-1.529801	2.145064
H	0.804433	-1.201412	2.906720
O	1.397081	-2.691559	-0.623532
H	1.716833	-3.495517	-0.176236
H	1.025837	-2.998461	-1.469817
H	2.035302	-0.882010	2.032654

0 imaginary frequencies

$E_{B3LYP-D3} = -904.677121$   
 $G_{B3LYP-D3} = -904.441988$   
 $E_{M06-2X-D3} = -904.532654$   
 $G_{tot} = -904.297522$

### 14

N	0.895566	-0.546200	0.170030
C	2.291270	-0.732454	-0.330439
C	2.381264	-2.266524	-0.430202
O	1.014384	-2.739107	-0.358233
C	0.207907	-1.716085	0.018847
C	0.091332	0.755230	-0.003935
H	2.363886	-0.280397	-1.324860
H	2.814977	-2.614048	-1.368463
O	-0.996963	-1.944630	0.182090
H	2.922106	-2.698911	0.416349
O	-1.004428	0.786576	0.698521
C	1.010358	1.987553	0.163459
C	0.356922	3.264522	-0.384396
C	1.362091	2.187093	1.646703

H	2.139451	2.953762	1.749697
H	1.924048	1.823766	-0.414705
C	3.416468	-0.215885	0.563955
H	3.288290	-0.570099	1.592541
H	4.362558	-0.618733	0.180610
H	-0.616348	3.446470	0.085520
H	1.002784	4.123152	-0.162599
H	1.726332	1.271398	2.121332
H	0.479208	2.523317	2.202809
O	-0.191740	0.566716	-1.522927
O	-1.352264	1.332188	-1.939163
H	-2.093003	0.740554	-1.661996
H	0.213628	3.220389	-1.467226
H	3.501176	0.871501	0.569024
Li	-2.261856	-0.558481	0.590874
O	-3.465842	-0.855431	2.097032
H	-4.387368	-0.600615	1.917712
O	-3.367643	-0.411444	-1.043094
H	-3.434509	-1.175638	-1.641758
H	-4.249939	-0.001895	-1.044042
H	-3.230366	-0.374787	2.909466

0 imaginary frequencies

$E_{B3LYP-D3} = -904.688638$

$G_{B3LYP-D3} = -904.452941$

$E_{M06-2X-D3} = -904.552019$

$G_{tot} = -904.316323$

## 15

N	2.752329	-0.121610	1.091081
C	3.327270	0.635135	-0.034293
C	2.562511	0.118913	-1.269807
O	1.383442	-0.495609	-0.701339
C	1.652943	-0.680337	0.676068
C	-1.971688	0.856775	-0.210528
H	3.104444	1.702688	0.110279
H	2.248116	0.903288	-1.962005
O	0.785276	-1.360251	1.311106
H	3.124530	-0.651526	-1.813029
O	-1.954643	-0.070689	0.582437
C	-1.602396	2.290203	0.091899
C	-2.548752	2.821359	1.184147
C	-0.128600	2.355480	0.529440
H	0.127613	3.394199	0.764277
H	-1.738083	2.877075	-0.821792
C	4.836660	0.477676	-0.167124
H	5.106621	-0.577152	-0.304905
H	5.206059	1.043245	-1.032479
H	-2.427421	2.251125	2.111596
H	-2.306730	3.870026	1.387048
H	0.539548	2.003172	-0.261729
H	0.037919	1.745740	1.423565
O	-2.327813	0.714519	-1.516960
O	-2.826423	-0.605345	-1.841207
H	-2.013469	-1.186543	-1.744051
H	-3.597072	2.762684	0.870504
H	5.349090	0.852597	0.726701
Li	-0.944255	-1.790948	0.687060
O	-1.939709	-3.172293	1.599937
H	-2.827413	-3.329046	1.233934
O	-0.698645	-2.136830	-1.271259
H	0.160238	-1.657002	-1.354564



H	-0.578656	-3.010402	-1.680104
H	-2.088438	-3.009282	2.547468

0 imaginary frequencies  
 $E_{\text{B3LYP-D3}} = -904.699222$   
 $G_{\text{B3LYP-D3}} = -904.467340$   
 $E_{\text{M06-2X-D3}} = -904.552062$   
 $G_{\text{tot}} = -904.320180$

## 16

N	-0.978671	-0.070509	-0.077014
C	-2.396047	0.002665	0.342471
C	-2.535485	-1.375829	0.990670
O	-1.672684	-2.214666	0.191323
C	-0.535511	-1.476031	-0.186220
C	-0.134694	0.960918	-0.309651
H	-2.522360	0.789526	1.088024
H	-2.193365	-1.374958	2.031583
O	-0.133055	-1.846840	-1.442712
H	-3.544784	-1.783963	0.926280
O	1.055235	0.757292	-0.642704
C	-0.633035	2.382171	-0.093681
C	-0.253596	2.802117	1.342229
C	-0.034564	3.336105	-1.133974
H	-0.428114	4.345605	-0.970502
H	-1.720870	2.411046	-0.184519
C	-3.344550	0.199873	-0.839999
H	-3.259569	-0.635319	-1.544050
H	-4.376905	0.247983	-0.475723
H	0.836054	2.822682	1.461442
H	-0.638580	3.808035	1.543740
H	-0.294117	3.027583	-2.153425
H	1.056648	3.376025	-1.052707
O	0.521905	-1.703612	0.758249
O	1.718620	-2.255703	0.081600
H	0.813183	-2.167602	-1.263552
H	-0.673674	2.117451	2.088172
H	-3.121618	1.128333	-1.375259
Li	2.380602	-0.468106	0.067864
O	4.025273	-0.312885	-1.006169
H	4.087812	0.540545	-1.469211
O	2.735170	0.403312	1.823118
H	1.908921	0.843829	2.088831
H	2.917812	-0.228616	2.539373
H	4.063592	-0.977414	-1.715688

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -904.685074$   
 $G_{\text{B3LYP-D3}} = -904.451081$   
 $E_{\text{M06-2X-D3}} = -904.547021$   
 $G_{\text{tot}} = -904.313028$

## 17

N	0.667621	-0.503983	0.415653
C	2.008427	-1.073949	0.081359
C	1.692595	-2.566138	0.071875
O	0.320378	-2.647587	-0.384702
C	-0.270787	-1.396627	-0.217257
C	0.288228	0.846499	-0.131894
H	2.304046	-0.767738	-0.930302
H	2.321725	-3.132506	-0.616773
O	-1.517778	-1.542088	0.411786
H	1.749932	-3.002531	1.075759

O	-0.844949	1.280781	0.373311
C	1.429937	1.883976	-0.183875
C	1.076137	3.034986	-1.139745
C	1.702444	2.435635	1.223762
H	1.880579	1.643737	1.957702
H	2.334221	1.401885	-0.565653
C	3.120041	-0.751829	1.072422
H	3.981469	-1.396213	0.856283
H	3.459336	0.283451	1.001343
H	0.143321	3.524395	-0.837004
H	1.873884	3.787261	-1.119489
H	0.851743	3.032238	1.572260
H	2.586556	3.084003	1.203564
O	-0.633397	-0.829868	-1.507369
O	0.102348	0.424716	-1.620699
H	-1.389698	-2.044463	1.237650
H	0.964599	2.691603	-2.173694
H	2.795399	-0.947529	2.100421
Li	-2.408778	0.300591	0.517854
O	-3.335303	0.108448	-1.235848
H	-2.518819	-0.208425	-1.674949
O	-3.596911	0.554064	2.021237
H	-4.325765	-0.085301	2.099567
H	-3.536336	0.958910	-1.661988
H	-3.160447	0.540287	2.890567

0 imaginary frequencies

$E_{B3LYP-D3} = -904.662014$

$G_{B3LYP-D3} = -904.424469$

$E_{M06-2X-D3} = -904.531109$

$G_{tot} = -904.293565$

## 18·19

N	2.094364	0.001219	0.953521
C	2.139628	1.206820	0.090211
C	2.614950	0.678069	-1.286139
O	2.545453	-0.779595	-1.146345
C	2.297785	-0.985722	0.170700
C	-1.552549	0.751285	-0.175281
H	1.121848	1.596421	0.004080
H	1.971299	0.961784	-2.119432
O	2.282558	-2.272775	0.557702
H	3.656064	0.933781	-1.505217
O	-1.913106	-0.075727	0.672430
C	-1.733655	2.249026	-0.041835
C	-3.198197	2.596943	-0.376352
C	-1.351427	2.716264	1.369372
H	-0.313095	2.463629	1.610940
H	-1.079293	2.729346	-0.777106
C	3.036128	2.300686	0.652251
H	3.050680	3.160260	-0.029138
H	2.666871	2.642984	1.625539
H	-3.881334	2.119414	0.335669
H	-3.338610	3.681833	-0.313267
H	-2.003012	2.257510	2.121208
H	-1.464373	3.804123	1.435051
O	-0.871413	-1.038961	-1.515587
O	-0.993234	0.403287	-1.328365
H	2.512405	-2.856169	-0.190830
H	-3.466089	2.272871	-1.388354
H	4.064393	1.938578	0.773354
Li	-1.544223	-1.896415	0.059371

O	-3.097164	-3.073151	-0.164867
H	-3.900661	-2.630596	-0.488171
O	-0.421641	-2.944070	1.263133
H	-0.548238	-3.905229	1.193266
H	-3.374874	-3.524309	0.651030
H	0.530535	-2.797796	1.086243

0 imaginary frequencies  
 $E_{\text{B3LYP-D3}} = -904.685252$   
 $G_{\text{B3LYP-D3}} = -904.453819$   
 $E_{\text{M06-2X-D3}} = -904.538111$   
 $G_{\text{tot}} = -904.306679$

## Reactions involving $\text{BnO}^-$

### $\text{BnO}^-$

O	-2.713079	-0.043983	0.778834
C	-2.032725	0.041985	-0.450138
C	2.266452	-0.024236	0.190114
C	1.590058	1.196815	0.085455
C	0.209458	1.216080	-0.146408
C	-0.519225	0.023530	-0.277222
C	0.173510	-1.194152	-0.173399
C	1.552650	-1.222357	0.059045
H	3.338925	-0.042807	0.368163
H	2.137284	2.132061	0.180511
H	-0.311178	2.168895	-0.228774
H	-0.376342	-2.128289	-0.276912
H	2.071629	-2.175472	0.132883
H	-2.295288	0.969126	-1.003886
H	-2.301473	-0.797647	-1.127334

0 imaginary frequencies  
 $E_{\text{B3LYP-D3}} = -346.317579$   
 $G_{\text{B3LYP-D3}} = -346.224714$   
 $E_{\text{M06-2X-D3}} = -346.234908$   
 $G_{\text{tot}} = -346.142043$

### TSL

N	0.711077	-0.543666	0.708745
C	-0.298773	-1.350805	1.440431
C	-1.086553	-0.239574	2.147688
O	-0.139476	0.842961	2.283412
C	0.759674	0.795967	1.246518
C	1.487823	-0.942992	-0.333800
H	-0.941984	-1.871841	0.730233
H	-1.941325	0.103862	1.562542
O	1.804401	1.474421	1.341699
H	-1.404438	-0.522257	3.151598
O	2.305659	-0.161177	-0.867631
C	1.369248	-2.366310	-0.857313
C	1.056960	-2.341743	-2.363344
C	2.687511	-3.109991	-0.571037
H	3.521653	-2.634058	-1.098521
H	0.557378	-2.888703	-0.349454
C	0.346965	-2.324113	2.425490
H	0.987105	-3.050414	1.916898
H	0.951887	-1.779869	3.159856
H	0.109040	-1.831676	-2.566700
H	0.979838	-3.370211	-2.733527
H	2.917008	-3.122259	0.500514
H	2.605416	-4.146020	-0.917872

H	1.851486	-1.833669	-2.920111
H	-0.440309	-2.870309	2.957334
C	-0.882848	1.156306	-1.197743
H	-0.304171	0.298306	-1.570572
O	-0.231097	1.785003	-0.108739
Li	2.842074	1.583360	-0.272465
O	1.814668	2.912889	-1.279613
H	1.940947	3.817607	-0.949514
O	4.749098	1.921074	-0.192071
H	4.982525	2.859784	-0.087669
H	0.970808	2.569516	-0.818776
H	5.209643	1.470272	0.536653
C	-2.296249	0.693858	-0.896794
C	-3.242576	1.594574	-0.382575
C	-2.680433	-0.636987	-1.107622
C	-4.537679	1.171529	-0.073778
H	-2.954495	2.629493	-0.211880
C	-3.977794	-1.066638	-0.803035
H	-1.953729	-1.346529	-1.497719
C	-4.909368	-0.163966	-0.280983
H	-5.258265	1.880160	0.327674
H	-4.255748	-2.105443	-0.964903
H	-5.915895	-0.495032	-0.037570
H	-0.919601	1.878814	-2.031425

1 imaginary frequency ( $244.3i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -1099.924989$

$G_{\text{B3LYP-D3}} = -1099.588247$

$E_{\text{M06-2X-D3}} = -1099.715297$

$G_{\text{tot}} = -1099.378555$

## TSM

N	-1.744585	-0.385391	-0.554771
C	-1.806592	-1.736345	-1.184309
C	-1.514412	-1.389411	-2.654707
O	-1.750315	0.042822	-2.754529
C	-1.733427	0.587549	-1.518429
C	-1.459088	-0.100593	0.832940
H	-1.007318	-2.359109	-0.783255
H	-0.475430	-1.572056	-2.938296
O	-1.722227	1.812808	-1.387218
H	-2.190468	-1.883484	-3.352366
O	-1.652808	1.066695	1.253044
C	-1.644439	-1.272394	1.799282
C	-0.716596	-1.191961	3.016908
C	-3.117103	-1.242757	2.273283
H	-3.271755	-0.399631	2.956151
H	-1.449682	-2.215860	1.284797
C	-3.158262	-2.427952	-1.020644
H	-3.157368	-3.338021	-1.631823
H	-3.970197	-1.778244	-1.367101
H	-0.769710	-0.202335	3.484887
H	0.321986	-1.390831	2.745062
H	-3.828310	-1.139384	1.448200
H	-3.348886	-2.168560	2.811544
H	-1.032872	-1.933966	3.760041
H	-3.351966	-2.719865	0.012840
C	1.265649	-0.927538	-0.162546
C	5.499621	-0.005870	-0.085422
C	4.681948	0.530595	-1.086940
C	3.319373	0.214258	-1.123011
C	2.754552	-0.638741	-0.163386

C	3.583688	-1.171065	0.835994
C	4.946540	-0.859613	0.877180
H	6.559202	0.235960	-0.056951
H	5.105074	1.191819	-1.839532
H	2.684922	0.633284	-1.901549
H	3.154850	-1.834672	1.584777
H	5.576899	-1.284124	1.655068
H	0.897062	-0.858438	-1.201064
H	1.101817	-1.967096	0.173415
O	0.587217	-0.026516	0.681121
Li	-1.139923	2.629152	0.280684
O	0.797375	2.493282	0.146834
H	1.312684	2.882937	0.871635
O	-1.892309	4.364012	0.674641
H	-1.517030	4.823061	1.445697
H	0.797982	1.478385	0.328736
H	-2.853801	4.376726	0.822116

1 imaginary frequency ( $144.0i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -1099.918343$

$G_{\text{B3LYP-D3}} = -1099.583546$

$E_{\text{M06-2X-D3}} = -1099.707768$

$G_{\text{tot}} = -1099.372972$

## TSN

N	-1.815778	0.030394	-0.197475
C	-2.505050	0.351465	-1.432956
C	-1.711011	1.522635	-2.041368
O	-1.230967	2.377982	-0.967419
C	-0.697951	1.804164	0.161155
C	-1.245232	-1.127543	0.117555
H	-2.491426	-0.464201	-2.165877
H	-0.868513	1.164811	-2.636066
O	-1.043724	2.224518	1.282782
H	-2.330414	2.175585	-2.659086
O	-0.651860	-1.215987	1.248432
C	-1.316545	-2.361283	-0.784096
C	-0.156922	-3.330267	-0.530868
C	-2.680505	-3.051484	-0.583993
H	-2.793394	-3.384479	0.455467
H	-1.255706	-2.023934	-1.825306
C	-3.959437	0.738055	-1.138532
H	-4.486579	-0.098769	-0.666703
H	-3.998032	1.596822	-0.457350
H	0.812668	-2.837729	-0.666929
H	-0.216704	-4.168923	-1.235276
H	-3.511837	-2.377811	-0.819483
H	-2.757045	-3.931270	-1.234189
H	-0.192157	-3.736212	0.486051
H	-4.484932	1.003572	-2.063753
C	1.186089	0.786964	-1.094810
C	5.149434	-0.511655	0.009542
C	4.985012	0.476559	-0.965549
C	3.699633	0.903524	-1.321117
C	2.572291	0.338897	-0.713489
C	2.742803	-0.656426	0.262905
C	4.024302	-1.076210	0.625207
H	6.146785	-0.841037	0.289640
H	5.853576	0.920503	-1.445211
H	3.572769	1.678877	-2.073236
H	1.868461	-1.096700	0.734657
H	4.146403	-1.845957	1.383123

H	1.213773	1.560064	-1.867243
H	0.587789	-0.059838	-1.444672
O	0.576414	1.323194	0.106372
Li	-0.886244	0.417123	2.351519
O	0.724553	0.410590	3.445977
H	0.973323	1.273720	3.819119
O	-2.912040	0.318412	2.403541
H	-3.284801	1.197518	2.585576
H	1.456288	0.183402	2.843845
H	-2.811595	0.293807	1.415676

1 imaginary frequency (190.0i cm<sup>-1</sup>)

E<sub>B3LYP-D3</sub> = -1099.908056  
G<sub>B3LYP-D3</sub> = -1099.572665  
E<sub>M06-2X-D3</sub> = -1099.700451  
G<sub>tot</sub> = -1099.365060

## TSO

N	-1.858007	-0.404843	-0.529116
C	-2.085086	-1.701093	-1.194348
C	-2.016376	-1.337217	-2.698490
O	-2.046616	0.113226	-2.729564
C	-1.842517	0.561420	-1.430196
C	-0.830886	-0.030472	1.102928
H	-1.273309	-2.391248	-0.943296
H	-1.086696	-1.665658	-3.173066
O	-1.678193	1.797685	-1.274119
H	-2.872351	-1.706774	-3.268022
O	-1.246078	1.081376	1.539154
C	-1.105715	-1.305323	1.909458
C	-0.033291	-1.444441	3.007139
C	-2.504954	-1.256833	2.531777
H	-2.549923	-0.501206	3.324351
H	-1.038237	-2.175214	1.251412
C	-3.415154	-2.348489	-0.807575
H	-3.559728	-3.268528	-1.387960
H	-4.251459	-1.670800	-1.019719
H	-0.029790	-0.563642	3.660737
H	0.971438	-1.565790	2.590310
H	-3.271348	-1.014764	1.790730
H	-2.749213	-2.229486	2.974411
H	-0.253664	-2.323138	3.624660
H	-3.435587	-2.610134	0.254053
C	1.059811	-0.978609	-0.232381
C	5.267846	-0.057508	-0.446111
C	4.377649	0.500125	-1.371437
C	3.016855	0.186119	-1.308143
C	2.532761	-0.684169	-0.320902
C	3.430095	-1.239185	0.602255
C	4.792278	-0.929167	0.540472
H	6.326785	0.183098	-0.495854
H	4.742951	1.175181	-2.141202
H	2.322503	0.617724	-2.025620
H	3.058506	-1.914688	1.369437
H	5.480710	-1.367316	1.258668
H	0.599548	-0.964452	-1.224351
H	0.879309	-1.949543	0.234706
O	0.463442	0.079938	0.559154
Li	-1.088267	2.589032	0.365396
O	0.888471	2.807171	0.080503
H	1.354549	3.220610	0.826377
O	-1.905979	4.264983	0.919186

H	-1.259114	4.946262	1.171939
H	1.010952	1.839847	0.211586
H	-2.506267	4.200464	1.682160

1 imaginary frequency (226.0i cm<sup>-1</sup>)  
E<sub>B3LYP-D3</sub> = -1099.922245  
G<sub>B3LYP-D3</sub> = -1099.586427  
E<sub>M06-2X-D3</sub> = -1099.715768  
G<sub>tot</sub> = -1099.379950

## 24

N	-0.600727	-0.813515	-0.452609
C	-0.403322	-2.067679	-1.203036
C	-0.292883	-1.523200	-2.628574
O	-1.119295	-0.345874	-2.643467
C	-1.192173	0.266002	-1.343748
C	-0.574494	-0.665707	0.883828
H	0.536862	-2.537964	-0.905558
H	0.741607	-1.271316	-2.883612
O	-2.395251	0.646316	-1.017602
H	-0.688951	-2.218730	-3.371673
O	-0.924157	0.417065	1.424674
C	-0.120194	-1.815852	1.774776
C	1.136989	-1.402672	2.556510
C	-1.269671	-2.198497	2.724231
H	-1.515342	-1.365033	3.391538
H	0.132144	-2.686821	1.167632
C	-1.576813	-3.039657	-1.049090
H	-1.725235	-3.334057	-0.006315
H	-2.502216	-2.579851	-1.413824
H	1.968684	-1.182888	1.881229
H	1.439430	-2.221214	3.220133
H	-2.174901	-2.474707	2.171057
H	-0.968514	-3.054384	3.338926
H	0.945657	-0.515499	3.169952
H	-1.380096	-3.943140	-1.637756
C	1.016877	1.400482	-1.832459
C	4.058361	0.340443	1.050614
C	3.931437	-0.395111	-0.131411
C	2.924069	-0.077132	-1.050611
C	2.039473	0.979628	-0.800905
C	2.164215	1.702961	0.395762
C	3.165471	1.386676	1.315952
H	4.839474	0.095243	1.765657
H	4.612871	-1.216309	-0.339433
H	2.829960	-0.648410	-1.971220
H	1.476054	2.519896	0.599118
H	3.251816	1.955292	2.238506
H	1.216057	2.432814	-2.138578
H	1.074003	0.778616	-2.728295
O	-0.337634	1.446984	-1.342564
Li	-2.350108	1.507809	0.685686
O	-1.380461	3.251995	0.441221
H	-1.899472	3.917261	-0.040939
O	-3.975178	1.708333	1.728606
H	-4.432208	2.559060	1.611100
H	-0.855790	2.784745	-0.252848
H	-4.654728	1.035910	1.548431

0 imaginary frequencies  
E<sub>B3LYP-D3</sub> = -1099.936181  
G<sub>B3LYP-D3</sub> = -1099.598198

$$E_{M06-2X-D3} = -1099.733911$$

$$G_{tot} = -1099.395928$$

## 25

N	2.178239	0.040259	0.428602
C	2.959052	-0.480663	-0.688876
C	2.033023	-1.024409	-1.784784
O	1.259290	-2.191152	-1.334586
C	0.450349	-2.206713	-0.263551
C	1.634116	1.239114	0.424505
H	3.557892	0.294637	-1.189053
H	1.359430	-0.252783	-2.155493
O	0.534468	-3.115783	0.555641
H	2.606559	-1.428463	-2.620853
O	0.825302	1.578187	1.381133
C	1.961783	2.316585	-0.621114
C	0.799546	3.286146	-0.864476
C	3.224557	3.072230	-0.158691
H	3.046813	3.565951	0.804987
H	2.191176	1.831599	-1.574736
C	3.920425	-1.558001	-0.177606
H	4.627367	-1.121546	0.536689
H	3.374171	-2.360151	0.330657
H	-0.097958	2.760235	-1.208347
H	1.081438	4.013130	-1.636369
H	4.078538	2.394564	-0.043410
H	3.495874	3.842976	-0.890551
H	0.541988	3.838716	0.045531
H	4.490693	-1.996026	-1.005324
C	-0.990302	-0.433629	-1.207227
C	-5.040328	0.600685	-0.166359
C	-4.767523	-0.619971	-0.795454
C	-3.455637	-0.947531	-1.148109
C	-2.406062	-0.059362	-0.874704
C	-2.684730	1.163883	-0.247513
C	-3.998220	1.494202	0.104497
H	-6.060803	0.855667	0.107350
H	-5.575610	-1.313944	-1.011405
H	-3.241072	-1.895753	-1.635865
H	-1.872345	1.852505	-0.030914
H	-4.204561	2.443751	0.591254
H	-0.918543	-0.988408	-2.145275
H	-0.348122	0.445647	-1.236354
O	-0.523399	-1.304020	-0.119159
Li	-0.018331	0.200930	2.340074
O	-1.877195	0.005056	2.771490
H	-2.134411	-0.911836	2.970586
O	1.353175	-1.127869	2.682978
H	1.042627	-2.025950	2.472518
H	-2.435382	0.258406	2.012946
H	1.788136	-0.798288	1.807766

0 imaginary frequencies

$$E_{B3LYP-D3} = -1099.921106$$

$$G_{B3LYP-D3} = -1099.584989$$

$$E_{M06-2X-D3} = -1099.708497$$

$$G_{tot} = -1099.372380$$

## 26

N	1.726909	0.355531	-0.501701
C	2.020401	1.665342	-1.147488
C	1.945496	1.288754	-2.638318



O	2.074598	-0.158668	-2.661039
C	1.773625	-0.636269	-1.418265
C	1.017483	0.116641	0.853825
H	1.231976	2.380326	-0.908440
H	0.982989	1.542937	-3.091277
O	1.598446	-1.855399	-1.275460
H	2.761699	1.705912	-3.228787
O	1.361403	-1.035304	1.391336
C	1.245993	1.340578	1.788141
C	0.170265	1.398486	2.883033
C	2.635956	1.256841	2.441637
H	2.642852	0.487647	3.222020
H	1.180733	2.267447	1.209666
C	3.379772	2.254690	-0.773001
H	3.569999	3.127229	-1.409436
H	4.180035	1.523918	-0.938655
H	0.119920	0.448636	3.429085
H	-0.823567	1.613431	2.480003
H	3.425226	1.006781	1.727339
H	2.889994	2.216113	2.908489
H	0.421040	2.186777	3.603539
H	3.411235	2.586586	0.266203
C	-1.072855	1.015812	-0.289525
C	-5.281357	0.053285	-0.310110
C	-4.431411	-0.485706	-1.283007
C	-3.072173	-0.157961	-1.282560
C	-2.547612	0.708302	-0.312512
C	-3.405781	1.244442	0.658281
C	-4.766150	0.920294	0.660717
H	-6.339004	-0.197974	-0.310494
H	-4.826644	-1.157561	-2.040843
H	-2.409778	-0.577204	-2.036754
H	-3.004411	1.917311	1.412813
H	-5.422866	1.344654	1.416080
H	-0.668202	0.989323	-1.308016
H	-0.890548	2.008561	0.137065
O	-0.434528	0.004751	0.513707
Li	1.034476	-2.595382	0.428721
O	-0.952572	-2.666942	0.145336
H	-1.457740	-2.988819	0.910362
O	1.798622	-4.303332	0.963004
H	1.141050	-4.977159	1.207720
H	-0.946269	-1.680858	0.242089
H	2.400827	-4.258638	1.725823

0 imaginary frequencies

$E_{B3LYP-D3} = -1099.928809$

$G_{B3LYP-D3} = -1099.590656$

$E_{M06-2X-D3} = -1099.726318$

$G_{tot} = -1099.388165$

**27**

N	-2.783812	1.546086	-0.288844
C	-1.930013	2.243824	-1.265892
C	-0.804912	2.845842	-0.405965
O	-0.834996	2.046361	0.799146
C	-2.089299	1.407668	0.805595
C	-0.711465	-1.580870	-0.449800
H	-1.502379	1.496894	-1.953365
H	0.189170	2.775909	-0.853048
O	-2.371950	0.774667	1.876202
H	-1.012226	3.889522	-0.133310

O	-1.425409	-1.835256	0.521289
C	-0.998657	-2.089737	-1.846211
C	-0.136366	-3.352294	-2.085497
C	-2.486173	-2.400971	-2.036007
H	-2.811886	-3.196615	-1.357789
H	-0.703364	-1.316212	-2.562347
C	-2.669144	3.285667	-2.094506
H	-1.979245	3.786138	-2.786442
H	-3.119949	4.048542	-1.446830
H	-0.434932	-4.148358	-1.393777
H	0.933416	-3.163227	-1.950225
H	-3.109515	-1.519086	-1.858676
H	-2.653278	-2.737884	-3.064951
H	-0.296496	-3.705707	-3.109532
H	-3.465747	2.820939	-2.687591
C	1.251828	-0.295899	-1.256958
C	4.984603	0.785031	0.606677
C	3.814671	1.487753	0.921534
C	2.605821	1.143733	0.312768
C	2.553234	0.089412	-0.612144
C	3.725521	-0.614177	-0.918435
C	4.938907	-0.265606	-0.315183
H	5.925888	1.055863	1.078072
H	3.845327	2.304593	1.638061
H	1.697477	1.684938	0.560136
H	3.687641	-1.434819	-1.631214
H	5.843477	-0.815032	-0.562733
H	0.708986	0.566626	-1.651061
H	1.415794	-1.025693	-2.048588
O	0.404433	-0.877942	-0.203466
Li	-1.456228	-0.837686	2.255550
O	0.466401	-0.572298	2.680431
H	0.883685	-1.330650	3.122546
O	-2.265049	-1.913074	3.661893
H	-1.871235	-2.797950	3.752917
H	0.822163	-0.586341	1.770381
H	-3.216167	-2.077852	3.540801

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -1099.937661$

$G_{\text{B3LYP-D3}} = -1099.605018$

$E_{\text{M06-2X-D3}} = -1099.725862$

$G_{\text{tot}} = -1099.393220$

## Reactions involving $\text{BnS}^-$

### $\text{BnS}^-$

S	-2.687233	-0.000058	-0.583088
C	-1.511763	0.000154	0.872372
C	2.640394	-0.000097	-0.375040
C	1.966143	1.208612	-0.161895
C	0.630249	1.205233	0.252977
C	-0.062866	0.000147	0.460359
C	0.630123	-1.205146	0.253112
C	1.965929	-1.208760	-0.161762
H	3.678949	-0.000276	-0.696641
H	2.481941	2.153992	-0.315127
H	0.113264	2.149194	0.415774
H	0.112897	-2.148937	0.416115
H	2.481721	-2.154148	-0.314960

H	-1.711137	-0.882749	1.491719
H	-1.711170	0.882999	1.491795

0 imaginary frequencies

$E_{B3LYP-D3} = -669.299920$   
 $G_{B3LYP-D3} = -669.209822$   
 $E_{M06-2X-D3} = -669.219861$   
 $G_{tot} = -669.129763$

### TSP

N	-0.711540	0.561640	0.727280
C	0.313771	1.284837	1.524355
C	0.906054	0.115251	2.316196
O	-0.208036	-0.782218	2.485636
C	-0.971675	-0.745353	1.326278
C	-1.341382	0.991920	-0.394882
H	1.066486	1.715605	0.865150
H	1.700306	-0.396191	1.761914
O	-2.124352	-1.249845	1.379439
H	1.255478	0.402003	3.308101
O	-2.188987	0.274864	-0.975724
C	-1.044457	2.378876	-0.946969
C	-0.745255	2.301304	-2.453072
C	-2.268087	3.280659	-0.683728
H	-3.144628	2.901892	-1.221596
H	-0.176550	2.807089	-0.441722
C	-0.298061	2.351770	2.430863
H	-0.784562	3.141537	1.852842
H	-1.036526	1.906935	3.107285
H	0.115362	1.658583	-2.664825
H	-0.522875	3.306279	-2.829079
H	-2.514853	3.333029	0.382103
H	-2.057523	4.295496	-1.039120
H	-1.609087	1.913059	-3.002913
H	0.497297	2.807087	3.032140
S	0.241359	-2.200084	-0.021381
C	1.115920	-1.241454	-1.341816
H	0.457431	-0.440849	-1.689867
Li	-3.119155	-1.236108	-0.250023
O	-2.582207	-2.836845	-1.258230
H	-2.618467	-2.717626	-2.222636
O	-5.048600	-1.032960	-0.121092
H	-5.528320	-1.279092	-0.930998
H	-1.616161	-2.738673	-1.018487
H	-5.330401	-0.120431	0.064475
C	2.455084	-0.674620	-0.934486
C	2.683282	0.708465	-0.951655
C	3.504203	-1.519246	-0.533863
C	3.920196	1.239919	-0.566884
H	1.884572	1.376847	-1.261464
C	4.741177	-0.995419	-0.152418
H	3.341402	-2.594394	-0.512370
C	4.953530	0.390115	-0.162919
H	4.071536	2.316689	-0.580530
H	5.540392	-1.665854	0.154611
H	5.914527	0.799010	0.138942
H	1.243306	-1.935941	-2.180986

1 imaginary frequency ( $158.1i \text{ cm}^{-1}$ )

$E_{B3LYP-D3} = -1422.901121$   
 $G_{B3LYP-D3} = -1422.569199$   
 $E_{M06-2X-D3} = -1422.692319$   
 $G_{tot} = -1422.360398$

## TSQ

N	1.443414	0.787952	-0.478170
C	1.250867	2.259769	-0.567015
C	0.399386	2.344414	-1.837514
O	0.760618	1.140734	-2.580181
C	1.227035	0.219592	-1.697963
C	1.544775	0.034341	0.769456
H	0.676578	2.583682	0.301398
H	-0.673001	2.296133	-1.631066
O	1.426228	-0.941373	-2.073400
H	0.633418	3.203182	-2.466116
O	1.571727	-1.227861	0.668612
C	2.450856	0.703571	1.812838
C	2.295161	0.090222	3.207135
C	3.912107	0.535499	1.337262
H	4.062791	0.879483	0.309720
H	2.208587	1.768933	1.869138
C	2.558963	3.039886	-0.696139
H	2.319070	4.094829	-0.873148
H	3.165395	2.980649	0.210040
H	1.284810	0.230899	3.600061
H	3.006615	0.562052	3.895267
H	4.581696	1.107756	1.989707
H	4.205757	-0.519660	1.387070
H	2.508471	-0.984869	3.186730
H	3.150739	2.672606	-1.542821
S	-0.653108	0.583013	1.632260
C	-1.468389	-0.583284	0.451088
C	-5.679715	0.294138	-0.035362
C	-5.255230	-0.597552	0.956666
C	-3.894555	-0.885663	1.107212
C	-2.934952	-0.288535	0.274127
C	-3.373364	0.600898	-0.720644
C	-4.732092	0.891433	-0.875854
H	-6.736833	0.517655	-0.155561
H	-5.983256	-1.071733	1.610753
H	-3.569941	-1.580959	1.878858
H	-2.640827	1.068002	-1.375838
H	-5.051868	1.579795	-1.654711
H	-1.334137	-1.606274	0.817000
H	-0.964594	-0.504035	-0.518271
Li	1.540884	-2.384737	-0.791446
O	-0.024920	-3.549519	-0.939971
H	-0.063021	-4.082010	-1.752794
O	3.123191	-3.514416	-0.923545
H	3.165601	-4.073219	-1.718448
H	-0.841081	-3.019657	-0.951075
H	3.952328	-3.005800	-0.934378

l imaginary frequency ( $136.9i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -1422.892781$

$G_{\text{B3LYP-D3}} = -1422.562212$

$E_{\text{M06-2X-D3}} = -1422.684560$

$G_{\text{tot}} = -1422.353991$

## TSR

N	1.634649	0.064300	-0.476201
C	2.221559	-0.230492	-1.764641
C	1.852733	-1.708566	-2.044383
O	1.927228	-2.449837	-0.800734
C	1.078560	-2.082473	0.188145

C	1.378573	1.242080	0.029011
H	1.777202	0.359582	-2.580781
H	0.850465	-1.811179	-2.468194
O	1.413579	-2.229186	1.367729
H	2.567602	-2.196796	-2.707551
O	0.904359	1.331229	1.232446
C	1.584421	2.551430	-0.738312
C	0.225856	3.236449	-0.969157
C	2.557392	3.474119	0.011395
H	2.154915	3.754977	0.991555
H	2.017895	2.325171	-1.717222
C	3.744238	-0.033811	-1.767667
H	3.998082	1.004440	-1.527567
H	4.214368	-0.682671	-1.018741
H	-0.462249	2.583595	-1.519396
H	0.363275	4.156335	-1.550922
H	3.527741	2.986395	0.166948
H	2.726203	4.393075	-0.563490
H	-0.247161	3.502133	-0.016934
H	4.164946	-0.276095	-2.751549
S	-0.751539	-2.152793	-0.103439
C	-1.296169	-0.837304	-1.315157
C	-4.888116	1.001473	0.218346
C	-3.629981	1.440646	0.651339
C	-2.469504	0.849097	0.149064
C	-2.550372	-0.189308	-0.793965
C	-3.812184	-0.623067	-1.223925
C	-4.976495	-0.030771	-0.721070
H	-5.791372	1.462487	0.609711
H	-3.553250	2.245750	1.378026
H	-1.494265	1.186315	0.488914
H	-3.882420	-1.425838	-1.954778
H	-5.948869	-0.375359	-1.063755
H	-1.457577	-1.309780	-2.286199
H	-0.478117	-0.121087	-1.380805
Li	0.944420	-0.289035	2.269665
O	-0.923353	-0.650947	2.855956
H	-1.436371	0.176041	2.840249
O	2.193182	-0.315341	3.766493
H	2.012981	0.381971	4.420415
H	-1.235549	-1.134157	2.062128
H	3.117328	-0.167947	3.500132

1 imaginary frequency ( $107.4i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -1422.869608$

$G_{\text{B3LYP-D3}} = -1422.539243$

$E_{\text{M06-2X-D3}} = -1422.655982$

$G_{\text{tot}} = -1422.325617$

## TSS

N	-1.156903	1.077026	0.273972
C	-0.753598	2.408344	-0.196360
C	0.248716	2.867243	0.887116
O	0.009993	1.964534	2.000845
C	-0.727637	0.892884	1.507264
C	-1.318365	-0.478241	-0.944454
H	-0.245697	2.310774	-1.162062
H	1.291145	2.751136	0.575366
O	-0.905048	-0.084916	2.279787
H	0.075454	3.887989	1.235251
O	-1.597854	-1.467904	-0.219168
C	-2.375975	0.083669	-1.909898

C	-2.519338	-0.843969	-3.132744
C	-3.729821	0.227330	-1.204246
H	-3.647139	0.826202	-0.293469
H	-2.037964	1.065714	-2.257075
C	-1.947465	3.355809	-0.336819
H	-1.605301	4.342387	-0.674077
H	-2.670963	2.975336	-1.064649
H	-1.599525	-0.899909	-3.723207
H	-3.316789	-0.466532	-3.783762
H	-4.447267	0.713534	-1.875551
H	-4.132283	-0.757478	-0.937804
H	-2.789402	-1.859782	-2.819584
H	-2.456286	3.477698	0.627735
S	0.398946	-0.438298	-1.694608
C	1.335870	-1.323743	-0.362447
C	5.312181	0.328704	0.006059
C	5.061387	-0.699016	-0.910086
C	3.776569	-1.240855	-1.022506
C	2.725885	-0.761876	-0.225381
C	2.987700	0.266776	0.693506
C	4.270944	0.807940	0.810198
H	6.310626	0.748983	0.096268
H	5.865204	-1.081203	-1.534489
H	3.585858	-2.042495	-1.733054
H	2.181643	0.640456	1.319582
H	4.458170	1.601355	1.529662
H	1.360496	-2.389966	-0.603622
H	0.770685	-1.192513	0.561337
Li	-1.761624	-1.670511	1.640583
O	-0.757337	-3.288783	2.121900
H	-0.553410	-3.385170	3.067980
O	-3.694590	-1.686187	2.039020
H	-3.925362	-1.312295	2.906724
H	0.111704	-3.225552	1.687333
H	-4.107176	-1.083489	1.395070

1 imaginary frequency ( $254.8i \text{ cm}^{-1}$ )

$E_{\text{B3LYP-D3}} = -1422.887288$

$G_{\text{B3LYP-D3}} = -1422.556578$

$E_{\text{M06-2X-D3}} = -1422.678095$

$G_{\text{tot}} = -1422.347385$

## 28

N	1.699047	-0.460212	-0.197928
C	2.360714	-1.601916	-0.874905
C	2.198866	-2.687571	0.197562
O	2.216931	-1.957821	1.432446
C	1.474007	-0.769738	1.243286
C	1.298483	0.695611	-0.772198
H	1.809088	-1.872926	-1.778148
H	1.248037	-3.225270	0.096879
O	1.685011	0.134174	2.125895
H	3.026842	-3.397324	0.213334
O	0.751590	1.604236	-0.100684
C	1.506383	0.914502	-2.266031
C	0.150431	1.175435	-2.944912
C	2.470921	2.096405	-2.469922
H	2.046635	3.018465	-2.057048
H	1.946386	0.026717	-2.721670
C	3.831393	-1.320972	-1.185977
H	3.951045	-0.458857	-1.848126
H	4.385066	-1.126004	-0.260584

H	-0.533026	0.329576	-2.813646
H	0.307272	1.328593	-4.018742
H	3.437047	1.913228	-1.985495
H	2.646319	2.247432	-3.541030
H	-0.328322	2.071292	-2.535865
H	4.269907	-2.197051	-1.677523
S	-0.519043	-1.370621	1.436024
C	-1.253571	-1.587113	-0.253790
C	-5.022236	0.513932	-0.570566
C	-3.812607	1.218310	-0.641083
C	-2.597140	0.538000	-0.547347
C	-2.566913	-0.857343	-0.381543
C	-3.781744	-1.553804	-0.313193
C	-5.002746	-0.874536	-0.407577
H	-5.968756	1.043489	-0.643803
H	-3.817089	2.297877	-0.771713
H	-1.662099	1.087718	-0.594704
H	-3.771921	-2.634198	-0.184748
H	-5.935167	-1.431163	-0.353500
H	-1.383064	-2.656440	-0.442563
H	-0.528375	-1.205441	-0.977405
Li	0.786610	1.783831	1.807055
O	-1.118349	1.618704	2.379177
H	-1.716881	2.091330	1.774910
O	1.599090	3.416752	2.488079
H	0.958981	4.118762	2.697060
H	-1.161268	0.675868	2.072812
H	2.225254	3.830670	1.869134

0 imaginary frequencies

$E_{B3LYP-D3} = -1422.903235$

$G_{B3LYP-D3} = -1422.569013$

$E_{M06-2X-D3} = -1422.695544$

$G_{tot} = -1422.361322$

## 29

N	1.675306	0.381155	-0.048910
C	2.378151	0.047751	-1.278504
C	1.795656	-1.225818	-1.899951
O	1.802013	-2.320386	-0.939183
C	0.780875	-2.747542	-0.210967
C	1.396372	1.621548	0.289067
H	2.247619	0.801835	-2.068034
H	0.793587	-1.084496	-2.295686
O	0.973165	-3.645483	0.603139
H	2.436131	-1.581326	-2.709609
O	0.869472	1.826901	1.460848
C	1.581447	2.832340	-0.631966
C	0.326708	2.959611	-1.519937
C	1.845244	4.128178	0.142436
H	0.987034	4.402669	0.765702
H	2.444221	2.651758	-1.282336
C	3.882413	-0.107808	-1.005539
H	4.285366	0.829900	-0.606579
H	4.062708	-0.899192	-0.267989
H	0.169198	2.060375	-2.126581
H	0.423377	3.817422	-2.196959
H	2.721622	4.032940	0.795011
H	2.031845	4.950257	-0.559785
H	-0.567881	3.111369	-0.902912
H	4.428506	-0.358922	-1.923716
S	-0.956532	-2.257787	-0.343758

C	-1.259497	-0.584927	-1.136458
C	-4.941529	0.930675	0.523919
C	-3.710411	1.323949	1.062306
C	-2.519376	0.830598	0.523792
C	-2.546346	-0.056282	-0.564598
C	-3.783355	-0.443752	-1.101705
C	-4.975714	0.046922	-0.560537
H	-5.867743	1.314821	0.943437
H	-3.677242	2.016598	1.899494
H	-1.563243	1.143682	0.935373
H	-3.809706	-1.126164	-1.948555
H	-5.928083	-0.257476	-0.986886
H	-1.324486	-0.723721	-2.217407
H	-0.420961	0.057427	-0.875529
Li	1.224128	-0.061392	1.882983
O	-0.351708	-0.935395	2.678055
H	-1.022330	-0.251068	2.849810
O	2.895177	-0.713948	2.667034
H	3.226415	-0.273819	3.468342
H	-0.751453	-1.478403	1.969099
H	3.571700	-0.541952	1.988560

0 imaginary frequencies

$E_{B3LYP-D3} = -1422.876851$

$G_{B3LYP-D3} = -1422.546221$

$E_{M06-2X-D3} = -1422.662656$

$G_{tot} = -1422.332026$

### 30

N	-0.509565	-0.664156	-0.670930
C	0.119250	-1.944858	-1.087304
C	1.281653	-1.408936	-1.926352
O	0.777095	-0.134986	-2.422725
C	-0.182343	0.303068	-1.549049
C	-1.325427	-0.444131	0.610992
H	0.480089	-2.463958	-0.198936
H	2.176875	-1.207733	-1.333594
O	-0.618647	1.457842	-1.684784
H	1.523157	-2.030222	-2.789043
O	-1.604203	0.811675	0.816138
C	-2.555121	-1.399004	0.590801
C	-3.380618	-1.312494	1.881222
C	-3.452285	-1.055432	-0.611642
H	-2.897213	-1.024616	-1.553781
H	-2.192238	-2.427917	0.485531
C	-0.796140	-2.850053	-1.917136
H	-0.219923	-3.726143	-2.237822
H	-1.660749	-3.203950	-1.352169
H	-2.808958	-1.619790	2.761812
H	-4.258384	-1.965577	1.801383
H	-4.249036	-1.802222	-0.711182
H	-3.926609	-0.077255	-0.465999
H	-3.736860	-0.288766	2.046060
H	-1.152362	-2.325799	-2.811685
S	-0.121036	-1.147644	2.066774
C	1.018733	0.289492	2.212325
C	4.389621	0.364914	-0.506802
C	4.290790	-0.637016	0.468639
C	3.198015	-0.664599	1.337535
C	2.185764	0.306279	1.253863
C	2.296803	1.305127	0.276870
C	3.388215	1.335457	-0.598985



H	5.237375	0.384519	-1.186991
H	5.065084	-1.396203	0.549661
H	3.122162	-1.448188	2.088378
H	1.519318	2.059316	0.193267
H	3.448947	2.113624	-1.355959
H	1.381295	0.261760	3.245730
H	0.410644	1.193365	2.099730
Li	-1.574615	2.295068	-0.247399
O	-0.536449	3.782573	0.547796
H	0.171787	4.062506	-0.057892
O	-3.360914	2.930049	-0.776613
H	-3.379233	3.571444	-1.507548
H	-0.062515	3.409962	1.312254
H	-3.881799	2.173933	-1.099247

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -1422.900299$

$G_{\text{B3LYP-D3}} = -1422.567205$

$E_{\text{M06-2X-D3}} = -1422.697116$

$G_{\text{tot}} = -1422.364022$

### 31

N	-2.051518	2.178038	-0.283921
C	-1.332243	3.011112	-1.263214
C	0.142174	2.937009	-0.804948
O	0.052420	2.474130	0.561681
C	-1.241999	1.944558	0.710802
C	-1.118123	-1.621524	-0.669674
H	-1.433107	2.576913	-2.264577
H	0.723219	2.205083	-1.377527
O	-1.446267	1.321654	1.803622
H	0.659230	3.900685	-0.812544
O	-1.464619	-1.661719	0.510169
C	-1.999502	-2.124501	-1.800561
C	-1.746769	-3.638942	-1.972214
C	-3.478267	-1.834902	-1.514557
H	-3.656166	-0.766829	-1.351901
H	-1.696936	-1.616138	-2.724318
C	-1.867015	4.443950	-1.297271
H	-1.330343	5.038617	-2.048055
H	-2.934350	4.456169	-1.548770
H	-0.698077	-3.850722	-2.206467
H	-2.366641	-4.016019	-2.793128
H	-4.082911	-2.159541	-2.368416
H	-3.817287	-2.382985	-0.628673
H	-2.017790	-4.178823	-1.057548
H	-1.737802	4.925546	-0.318976
S	0.481827	-1.040185	-1.161015
C	1.294972	-0.798273	0.488689
C	5.494241	0.004559	-0.114075
C	5.038055	-1.315119	-0.013051
C	3.678562	-1.572899	0.183706
C	2.760279	-0.516558	0.285359
C	3.224376	0.803585	0.182201
C	4.584153	1.062825	-0.015078
H	6.551536	0.206176	-0.265746
H	5.739886	-2.142146	-0.084626
H	3.324513	-2.598456	0.263322
H	2.518391	1.625629	0.262381
H	4.931848	2.090138	-0.088683
H	1.134847	-1.717988	1.057187
H	0.791890	0.029166	0.990058

Li	-1.868907	-0.494992	2.031176
O	-0.809973	-1.308357	3.476677
H	-0.808675	-0.795301	4.303082
O	-3.806867	-0.849614	2.182210
H	-4.318538	-0.066185	2.448457
H	0.123538	-1.332603	3.201555
H	-4.137075	-1.066751	1.292514

0 imaginary frequencies

$E_{\text{B3LYP-D3}} = -1422.902712$

$G_{\text{B3LYP-D3}} = -1422.574571$

$E_{\text{M06-2X-D3}} = -1422.688958$

$G_{\text{tot}} = -1422.360817$