1a.MeO(−)Me
SCF Energy: −3227.54806789

C	3.939720	1.360195	−1.792636
C	3.314962	1.007941	−0.456492
C	2.072222	1.265628	−0.108951
C	1.084416	1.281364	0.834163
C	0.032410	0.089691	0.756024
O	0.528865	−0.991850	−0.091825
C	1.570777	−1.769180	0.233761
C	1.977874	−2.584374	−0.977893
O	0.799123	2.193882	1.660602
C	−1.224453	0.568690	0.043080
Br	−2.490115	−0.874310	−0.471730
C	−0.314303	−0.382111	2.172716
C	−1.571775	1.832212	−0.161293
C	−2.813604	2.393663	−0.776621
O	2.121030	−1.845353	1.305992
H	4.791172	2.047497	−1.676061
H	4.331583	0.473373	−2.314096
H	3.204482	1.839917	−2.444201
H	4.008960	0.506572	0.237652
H	−0.677882	0.486292	2.720600
H	−3.500969	1.620930	−1.120662
H	−3.344070	3.031455	−0.058677
H	−2.558453	3.033714	−1.629687
H	−0.843058	2.547587	0.218031
H	0.573388	−0.765425	2.669171
H	−1.083311	−1.159121	2.152758
H	1.103011	−2.978943	−1.497896
H	2.508192	−1.924817	−1.669451
H	2.639364	−3.393931	−0.670240

1a.MeOLiMe
SCF Energy: −3235.10733260

C	1.420318	3.748976	−1.317509
C	1.939177	2.334558	−1.187583
C	1.693700	1.511435	−0.201266
C	1.426271	0.734799	0.846070
O	2.140470	0.649399	1.949352
Li	3.319022	−0.489232	1.341389
C	0.248007	−0.289243	0.715603
C	−1.076157	0.351436	0.326920
C	−1.392053	1.627525	0.532898
C	−2.695297	2.326961	0.315274
C	0.075627	−1.123955	1.984810
O	0.543174	−1.240396	−0.413498
C	1.686168	−1.867685	−0.559878
O	2.667281	−1.774267	0.177611
C	1.703353	−2.730725	−1.794039
H	2.248116	4.461072	−1.411212
H	0.803455	3.861372	−2.216811
H	0.822415	4.039607	−0.452249
H	2.574253	2.007957	−2.017936
H	−0.119546	−0.457683	2.824232
H	−3.474015	1.666811	−0.062473
H	−3.045349	2.773925	1.252286
H	−2.567056	3.152150	−0.393670
H	−0.583761	2.245239	0.913199
Br	−2.428184	−0.880559	−0.339873
H	0.977915	−1.687269	2.215557
H	−0.759556	−1.815764	1.869621
H	0.699592	−3.043602	−2.075758
H	2.122668	−2.145324	−2.618155
H	2.348148	−3.593599	−1.630786

1a.tsE.MeO(−)Me
SCF Energy: −3227.51732904

C	2.986808	0.672562	1.127843
C	1.616117	0.084441	1.325969
C	0.427084	0.672221	0.939876
C	−0.699546	−0.330101	0.801995
C	−0.120661	−1.360509	−0.245788
O	−0.901041	−1.929588	−1.018365
Br	0.520236	2.051824	−0.458967
C	−1.045969	−0.991351	2.144264
O	−1.848792	0.307704	0.202736
C	−3.006406	−0.332189	−0.067116
C	−3.626185	0.264886	−1.312636
O	−3.532192	−1.197099	0.590420
C	1.293498	−1.534372	−0.121071
C	2.148804	−1.743697	−1.125060
C	3.593195	−2.150794	−0.982094
H	3.842246	−2.343116	0.065430
H	3.810913	−3.065519	−1.554355
H	4.287325	−1.384558	−1.358445
H	1.807524	−1.626083	−2.165424
H	1.539116	−0.573647	2.181258
H	3.757407	−0.040337	1.430054
H	3.109686	1.581695	1.729928
H	3.159001	0.940633	0.085285
H	−1.832760	−1.726805	2.000479
H	−0.171099	−1.493278	2.556579
H	−1.388023	−0.233395	2.857038
H	−3.497131	1.348377	−1.335773
H	−4.681778	−0.001411	−1.371151
H	−3.094905	−0.151118	−2.172484

1a.tsE.MeOLiMe
SCF Energy: −3235.04755478

C	2.920262	1.003134	1.012035
C	1.617977	0.273164	1.216758
C	0.394100	0.722805	0.736894
C	−0.715047	−0.313156	0.786005
C	0.023379	−1.390309	−0.054460
O	−0.610659	−2.271410	−0.729523
Br	0.301234	2.166230	−0.504935
C	−1.101553	−0.737912	2.205961
O	−1.838286	0.177414	0.032342
C	−3.019871	−0.489263	−0.081798
C	−3.878183	0.215157	−1.106651
O	−3.345917	−1.469276	0.529728
C	1.415411	−1.268682	−0.029573
C	2.365616	−1.587870	−0.958269
C	3.818095	−1.888704	−0.659387
H	3.948844	−2.201053	0.379627
H	4.209267	−2.690055	−1.298136
H	4.468760	−1.021728	−0.827655
H	2.162097	−1.337157	−2.016215
H	1.576731	−0.293181	2.140040
H	3.758657	0.393979	1.352833
H	2.928541	1.934843	1.586267
H	3.081480	1.259523	−0.035331
H	−1.751169	−1.608103	2.179452
H	−0.212599	−0.976965	2.790054
H	−1.625571	0.082889	2.703427
H	−3.883910	1.292816	−0.935996
H	−4.890631	−0.182172	−1.066534
H	−3.461504	0.044940	−2.102870
Li	0.821869	−3.080211	−1.413905

1a.tsE.PhO(−)tBu
SCF Energy: −3537.25577468

C	−1.784652	−1.169358	0.673794
C	−0.461994	−0.585674	1.020892
C	0.782529	−1.038677	0.570340
Br	0.950117	−1.998946	−1.125448
C	1.869510	−0.030812	0.865624
O	3.093795	−0.422956	0.214962
C	4.221975	0.319631	0.234871
O	4.608438	1.035444	1.125542
C	1.302535	1.240335	0.123338
C	−0.126959	1.372299	0.256950
C	−0.862154	2.100795	−0.591874
C	−2.247532	2.703823	−0.393516
C	2.076119	0.191609	2.371709
O	2.084498	1.994712	−0.460309
C	5.006940	0.061440	−1.033391
C	−2.870033	2.313662	0.953823
C	−2.080773	4.241701	−0.439707
C	−3.188213	2.287111	−1.544000
H	−0.389679	2.429258	−1.532232
H	−0.443912	−0.277951	2.058932
H	2.845835	0.941793	2.531244
H	1.154400	0.535886	2.839376
H	2.382854	−0.747346	2.844961
H	4.969504	−0.993018	−1.312113
H	6.037903	0.392357	−0.907989
H	4.534688	0.633772	−1.835942
H	−3.049622	4.749406	−0.347987
H	−1.433762	4.585075	0.372150
H	−1.622876	4.559861	−1.382036
H	−4.156403	2.798784	−1.471140
H	−2.750152	2.538842	−2.515960
H	−3.373223	1.211039	−1.528874
H	−3.827423	2.828721	1.103035
H	−3.051108	1.239880	1.013813
H	−2.202891	2.580496	1.777427
C	−2.605701	−1.639075	1.710167
C	−3.854148	−2.200682	1.454021
C	−4.318727	−2.296970	0.144233
C	−3.521601	−1.821925	−0.896478
C	−2.272785	−1.263368	−0.636852
H	−2.251114	−1.566369	2.734690
H	−4.463983	−2.560263	2.278638
H	−5.292985	−2.731054	−0.063369
H	−3.877303	−1.879803	−1.921609
H	−1.672706	−0.879058	−1.449560

1a.tsZ.MeO(−)Me
SCF Energy: −3227.51982649

C	2.083240	−0.109988	2.331692
C	0.783321	−0.012246	1.585231
C	0.460652	−0.685831	0.432394
Br	1.801007	−1.793676	−0.443137
C	−0.684732	−0.142394	−0.343658
C	−0.918203	−0.685496	−1.742397
O	−1.913536	−0.363387	0.562693
C	−3.195321	−0.339269	0.199559
O	−3.667612	−0.490049	−0.904143
C	−0.472500	1.410654	−0.372352
C	0.597099	1.855883	0.434039
C	1.641922	2.671462	0.354254
C	2.246611	3.195982	−0.932715
C	−4.062672	−0.108283	1.431221
O	−1.266728	2.115615	−1.022514

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H         1.591406    2.983894   -1.780173
H         2.399200    4.283972   -0.890804
H         3.230672    2.750687   -1.143566
H         2.154958    3.002656    1.266315
H        -0.062366    0.303695    2.181349
H         2.156326   -1.057327    2.881261
H         2.165602    0.703908    3.056747
H         2.939074   -0.052854    1.656959
H        -1.721675   -0.130083   -2.214317
H        -0.004261   -0.558129   -2.326494
H        -1.172498   -1.747260   -1.724442
H        -3.704745   -0.693934    2.280196
H        -5.099476   -0.358655    1.205412
H        -4.000976    0.947784    1.709452

1a.tsZ.MeOLiMe
SCF Energy: -3235.05254807
C         1.854298   -0.225996    2.429472
C         0.605359   -0.180162    1.596086
C         0.446239   -0.783899    0.362507
C        -0.764260   -0.342620   -0.412311
C        -0.452778    1.168161   -0.442412
O        -0.938331    1.966587   -1.319030
C        -0.994956   -0.926307   -1.794634
O        -1.910173   -0.674123    0.475068
C        -3.171516   -0.247464    0.228772
C        -4.094904   -0.743825    1.321846
O        -3.516662    0.427537   -0.704456
C         0.428238    1.579267    0.559742
C         1.363705    2.558218    0.668398
C         2.366304    2.913403   -0.427745
Li       -0.213480    3.450512   -0.642311
H         2.039577    2.570122   -1.415666
H         2.569763    3.991389   -0.480936
H         3.336914    2.436104   -0.247180
H         1.610938    2.955193    1.654923
Br        1.896694   -1.660669   -0.521244
H        -0.313062   -0.044511    2.153577
H         1.943653   -1.193782    2.934111
H         1.824593    0.546523    3.200713
H         2.753691   -0.080379    1.829924
H        -1.853051   -0.436368   -2.247985
H        -0.126884   -0.760404   -2.432768
H        -1.175005   -2.000951   -1.725295
H        -3.954466   -1.812665    1.491742
H        -5.127103   -0.539029    1.043686
H        -3.866454   -0.232044    2.260640

1a.tsZ.PhO(-)tBu
SCF Energy: -3537.26177442
C        -1.642274   -1.516395   -0.639691
C        -0.236986   -1.074661   -0.484277
C         0.584986   -0.967344    0.631712
C         1.850010   -0.223920    0.315028
C         1.391053    1.044359   -0.484630
O         2.217006    1.933335   -0.759051
Br       -0.149003   -0.756671    2.424430
C         2.770339    0.148963    1.463826
O         2.558153   -1.132215   -0.687484
C         3.830508   -1.051449   -1.088618
C         4.017131   -1.923080   -2.323785
O         4.735586   -0.423850   -0.593203
C         0.026644    1.009619   -0.859795
C        -1.038731    1.797019   -0.942409
C        -1.291701    3.150649   -0.270011
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C       -0.257480    3.464255    0.819289
C       -1.224380    4.241120   -1.362810
C       -2.704983    3.146904    0.348900
H       -1.884437    1.486780   -1.569426
H        0.338792   -1.306255   -1.371717
H        3.602230    0.731263    1.082874
H        2.219154    0.749205    2.188651
H        3.148562   -0.742948    1.969350
H        3.513844   -2.884402   -2.205597
H        5.080725   -2.070439   -2.510438
H        3.568734   -1.420499   -3.185649
H       -0.468655    4.438224    1.278646
H       -0.281815    2.706284    1.606968
H        0.752402    3.482818    0.407616
H       -1.454314    5.232684   -0.951239
H       -0.224990    4.273314   -1.803327
H       -1.940311    4.039357   -2.167498
H       -2.950165    4.123555    0.785119
H       -3.467739    2.916716   -0.403289
H       -2.781031    2.393013    1.137338
C       -2.274794   -1.258207   -1.869299
C       -3.572362   -1.686344   -2.124623
C       -4.279855   -2.396908   -1.154795
C       -3.664363   -2.674081    0.063058
C       -2.364033   -2.241546    0.319493
H       -1.727234   -0.704628   -2.625309
H       -4.033309   -1.463525   -3.083219
H       -5.295326   -2.731631   -1.348244
H       -4.197310   -3.237145    0.824915
H       -1.901040   -2.480124    1.266941

1b.MeO(-)Me
SCF Energy: -3227.53932697
C       -3.255714    2.350271   -1.647080
C       -2.202470    2.292580   -0.559444
C       -1.935269    1.256444    0.199485
C       -1.308853    0.570747    1.190914
C       -0.111084   -0.379962    0.707091
C        0.306013   -1.320456    1.841633
O       -1.625829    0.471015    2.411746
O       -0.453891   -1.155591   -0.487276
C       -1.586492   -1.872997   -0.660695
C       -2.534595   -2.137799    0.496519
C        1.083693    0.457582    0.278765
C        1.241709    1.759817    0.490762
C        2.408579    2.642760    0.176624
O       -1.783217   -2.364274   -1.747551
H       -3.780481    1.395408   -1.726108
H       -2.814082    2.576840   -2.628120
H       -4.000113    3.136382   -1.451121
H       -1.641620    3.238764   -0.449340
H        1.091083   -1.999386    1.501857
H        0.668731   -0.731587    2.683488
H       -0.544621   -1.894493    2.202779
H        0.383148    2.246761    0.945458
Br       2.546826   -0.549724   -0.576127
H        2.724544    3.193227    1.070730
H        3.264511    2.089090   -0.208097
H        2.124205    3.395113   -0.568831
H       -2.505236   -1.413193    1.306104
H       -3.541936   -2.186437    0.083064
H       -2.296649   -3.129261    0.899792

1b.MeOLiMe
SCF Energy: -3235.10781731
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C       -2.916468    2.279267   -1.997094
C       -1.968033    2.454391   -0.833791
C       -1.669024    1.551872    0.063540
C       -1.280322    0.755464    1.058337
O       -1.883958    0.617718    2.218889
Li      -3.088379   -0.526317    1.671968
C       -0.087868   -0.224963    0.788772
C        1.166124    0.476949    0.289494
C        1.443170    1.764766    0.477941
C        2.685936    2.524253    0.140716
C        0.235355   -1.075555    2.017257
O       -0.453991   -1.165728   -0.326832
C       -1.583490   -1.831445   -0.380676
O       -2.498019   -1.778992    0.441193
C       -1.679266   -2.680025   -1.621038
H       -3.365696    1.283706   -2.001505
H       -2.399748    2.425007   -2.952960
H       -3.725216    3.018310   -1.960677
H       -1.504329    3.445492   -0.770386
H        1.082355   -1.730265    1.809096
H        0.482660   -0.417919    2.849689
H       -0.619472   -1.678857    2.317696
H        0.648412    2.344916    0.938334
Br       2.497873   -0.687978   -0.522860
H        3.080787    3.019534    1.034329
H        3.468690    1.895110   -0.279420
H        2.457669    3.318143   -0.579150
H       -0.694258   -2.978133   -1.976000
H       -2.302038   -3.551892   -1.424391
H       -2.159182   -2.088806   -2.407215

1b.tsE.MeO(-)Me
SCF Energy: -3227.51958790
C       -2.202966    0.444654    1.980149
C       -0.850928    0.370614    1.326208
C       -0.415561   -0.642012    0.503012
Br      -1.704012   -1.947900   -0.152703
C        0.775365   -0.313698   -0.337542
C        1.199713   -1.314654   -1.396207
O        1.887507   -0.083236    0.689166
C        3.197076   -0.004933    0.447741
O        3.800984   -0.336268   -0.545448
C        0.453948    1.087168   -0.970229
C       -0.647145    1.750510   -0.367564
C       -1.690119    2.417163   -0.854634
C       -2.585587    3.352594   -0.078998
C        3.894318    0.581072    1.669930
O        1.181740    1.523840   -1.876055
H       -2.210823    3.499611    0.937713
H       -2.643896    4.340791   -0.559780
H       -3.620779    2.987065   -0.005825
H       -2.339990    1.408494    2.475517
H       -3.006232    0.318180    1.252426
H       -2.316503   -0.342642    2.736156
H       -0.058593    0.892581    1.844914
H        0.357683   -1.508309   -2.062775
H        1.509241   -2.261132   -0.945827
H        2.018411   -0.899024   -1.973691
H        3.492828    0.157770    2.592469
H        4.967142    0.399940    1.602505
H        3.714976    1.659847    1.697000
H       -1.953599    2.317752   -1.918693

1b.tsE.MeOLiMe
SCF Energy: -3235.05397162
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C       -2.036808    0.532557    2.085918
C       -0.722561    0.287257    1.397350
C       -0.497276   -0.714788    0.469496
C        0.784248   -0.586362   -0.305131
C        0.495785    0.798164   -0.922686
O        0.982200    1.168337   -2.044843
C        1.125601   -1.639388   -1.342483
O        1.840482   -0.559994    0.735330
C        3.095469   -0.126724    0.471549
C        3.937322   -0.216598    1.726628
O        3.486926    0.277124   -0.591386
C       -0.396183    1.577170   -0.171259
C       -1.316355    2.505292   -0.545430
C       -1.889639    3.584540    0.345906
Li       0.267506    2.795371   -2.069189
H       -1.238789    3.770611    1.203402
H       -2.016341    4.533521   -0.189145
H       -2.880538    3.319034    0.733825
H       -2.011922    1.470266    2.643141
H       -2.866456    0.570476    1.378833
H       -2.248481   -0.271405    2.798650
H        0.155322    0.585697    1.955497
Br      -1.937253   -1.754162   -0.234805
H        0.330878   -1.728194   -2.082719
H        1.266223   -2.609206   -0.861427
H        2.037562   -1.345309   -1.857861
H        3.855116   -1.207624    2.176546
H        4.975566    0.000169    1.482371
H        3.581032    0.506269    2.465387
H       -1.892328    2.324788   -1.472711

1b.tsE.PhO(-)tBu
SCF Energy: -3537.25960585
C       -1.497219   -1.026588    0.821114
C       -0.143112   -0.450451    0.654430
C        0.849228   -0.953830   -0.180903
C        2.024758   -0.084930   -0.373163
C        1.394493    1.287566   -0.763170
O        2.096130    2.152649   -1.303814
Br       0.611576   -2.527117   -1.279760
C        3.093934   -0.516968   -1.356452
O        2.639851    0.070941    1.049684
C        3.803002    0.647708    1.351061
C        3.899152    0.828359    2.862518
O        4.685621    0.993497    0.600548
C        0.019264    1.439096   -0.395798
C       -0.933445    2.140365   -1.009391
C       -2.201682    2.767249   -0.440531
C       -2.359470    2.505358    1.063471
C       -2.096665    4.293538   -0.669682
C       -3.446798    2.250289   -1.192091
H        0.226454    0.016687    1.558272
H        2.634229   -0.712961   -2.326996
H        3.593111   -1.429173   -1.020743
H        3.819839    0.281981   -1.465074
H        3.559709   -0.066952    3.386833
H        4.926834    1.064273    3.138923
H        3.248764    1.653691    3.166538
H       -0.761127    2.426654   -2.059187
H       -2.996539    4.810799   -0.312737
H       -1.230866    4.705032   -0.143818
H       -1.975864    4.525550   -1.733064
H       -4.355557    2.771877   -0.864873
H       -3.343306    2.406641   -2.271465
H       -3.590905    1.181310   -1.021060
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H       -3.231443    3.039954    1.460365
H       -2.491915    1.443617    1.272600
H       -1.472725    2.841426    1.607295
C       -1.978163   -1.297795    2.110598
C       -3.244566   -1.840485    2.313769
C       -4.070015   -2.112749    1.224752
C       -3.614328   -1.831399   -0.063264
C       -2.345939   -1.294730   -0.262947
H       -1.341006   -1.082869    2.963967
H       -3.587744   -2.047326    3.323982
H       -5.060860   -2.531569    1.377482
H       -4.254682   -2.025003   -0.919493
H       -2.006948   -1.058848   -1.263417

1b.tsZ.MeO(-)Me
SCF Energy: -3227.51630305
C        3.114894   -0.421099    1.242718
C        1.661642   -0.104773    1.465447
C        0.591935   -0.752098    0.884389
Br       0.929378   -1.837390   -0.714440
C       -0.674214    0.079125    0.893131
C       -1.200835    0.318888    2.314730
O       -1.666679   -0.543306    0.043926
C       -2.925066   -0.084712   -0.113774
O       -3.625858    0.430549    0.722788
C       -0.231196    1.421105    0.180882
C        1.138925    1.726066    0.384829
C        2.059152    2.285583   -0.404066
C        1.927822    2.505219   -1.896670
C       -3.391741   -0.386780   -1.522445
O       -1.100019    2.090192   -0.404203
H        0.909009    2.296589   -2.226346
H        2.163357    3.545034   -2.167131
H        2.616208    1.870975   -2.474612
H        3.387986   -1.369168    1.723717
H        3.348493   -0.506834    0.181284
H        3.742619    0.366138    1.667791
H        1.455319    0.346233    2.427593
H       -0.413617    0.735970    2.942837
H       -1.537087   -0.625174    2.755602
H       -2.034199    1.015801    2.291611
H       -3.039287   -1.364910   -1.854136
H       -4.478961   -0.326983   -1.577991
H       -2.950564    0.366332   -2.180586
H        3.015035    2.620026    0.020644

1b.tsZ.MeOLiMe
SCF Energy: -3235.04655062
C        3.072447   -0.640916    1.169388
C        1.661937   -0.156124    1.373154
C        0.547947   -0.705638    0.755531
Br       0.710437   -2.058206   -0.576815
C       -0.710977    0.139199    0.854868
C       -1.271771    0.254237    2.275005
O       -1.676540   -0.371176   -0.086764
C       -2.951341    0.093415   -0.194954
O       -3.492988    0.867459    0.545307
C       -0.103559    1.444793    0.272561
C        1.285082    1.493587    0.331292
C        2.254323    2.109690   -0.406748
C        2.316253    2.065471   -1.932295
C       -3.596212   -0.536526   -1.408204
O       -0.834686    2.375114   -0.219258
H        1.335829    1.868491   -2.381738
H        2.719154    2.990882   -2.364761
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H         2.973820    1.260492   -2.283559
H         3.232957   -1.588631    1.692966
H         3.299152   -0.801012    0.114995
H         3.784260    0.084495    1.568648
H         1.491013    0.281314    2.351046
H        -0.472493    0.491448    2.978380
H        -1.715800   -0.698900    2.574815
H        -2.031665    1.028697    2.326649
H        -3.419738   -1.613120   -1.428154
H        -4.664024   -0.326178   -1.401219
H        -3.150230   -0.116169   -2.313408
H         3.189494    2.400596    0.075737
Li        0.523974    3.478833   -0.591245

1b.tsZ.PhO(-)Me
SCF Energy: -3537.25702717
C        -2.274474   -1.068701   -0.659750
C        -0.827283   -0.982199   -0.975377
C         0.291072   -1.392848   -0.250699
C         1.550893   -0.831877   -0.897029
C         1.243492    0.711097   -1.064442
O         2.194780    1.485598   -1.262559
Br        0.246647   -1.340921    1.712794
C         1.880558   -1.514395   -2.231030
O         2.648754   -0.927688    0.046568
C         3.949985   -0.735976   -0.235474
C         4.678254   -0.379215    1.045770
O         4.502332   -0.854111   -1.300878
C        -0.137772    1.016670   -1.023692
C        -0.925182    1.995137   -0.581953
C        -0.620709    3.119860    0.413585
C         0.639092    2.847910    1.246898
C        -0.421999    4.422781   -0.394626
C        -1.830277    3.292836    1.355185
H        -0.683136   -1.092868   -2.043630
H         0.997330   -1.547307   -2.870252
H         2.210309   -2.542166   -2.055073
H         2.667928   -0.973012   -2.748290
H         4.320218   -0.980425    1.882930
H         5.751675   -0.508452    0.908404
H         4.466590    0.668111    1.277789
H        -1.953877    2.056706   -0.959167
H         0.805061    3.662814    1.963441
H         0.542116    1.914228    1.806812
H         1.517386    2.761048    0.606920
H        -0.257331    5.280934    0.270332
H         0.441994    4.326362   -1.056125
H        -1.298851    4.643246   -1.013674
H        -1.678930    4.134003    2.043123
H        -2.749912    3.484754    0.791067
H        -1.991090    2.390324    1.951424
C        -3.172849   -0.382828   -1.495693
C        -4.548197   -0.465481   -1.309234
C        -5.070096   -1.246787   -0.278346
C        -4.194953   -1.944186    0.550459
C        -2.816039   -1.859610    0.363253
H        -2.770676    0.226375   -2.298922
H        -5.214590    0.082743   -1.969923
H        -6.144034   -1.312460   -0.126442
H        -4.585452   -2.567134    1.351027
H        -2.153378   -2.419098    1.008568

1b.tsZ.int.MeO(-)Me
SCF Energy: -3227.55838481
C         3.002284   -0.736018    1.210499
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C         1.676570    0.019485    1.242652
C         0.391009   -0.854427    1.176778
Br        0.573271   -1.993153   -0.660320
C        -0.660989    0.239622    0.883421
C        -0.986593    0.953800    2.209605
O        -1.855164   -0.337527    0.305350
C        -2.948354    0.365771   -0.017069
O        -3.247693    1.478174    0.349984
C         0.038741    1.158859   -0.137574
C         1.501388    1.109600    0.187566
C         2.471520    1.785407   -0.446320
C         2.321291    2.721389   -1.611770
C        -3.818743   -0.474484   -0.932107
O        -0.494402    1.674531   -1.104439
H         1.277170    2.856228   -1.883042
H         2.768938    3.699291   -1.387568
H         2.854515    2.333483   -2.490236
H         2.963072   -1.560436    1.928234
H         3.187847   -1.159772    0.222571
H         3.845645   -0.087764    1.478391
H         1.617424    0.478735    2.241417
H        -0.120172    1.498236    2.587827
H        -1.257704    0.194369    2.949126
H        -1.804657    1.656744    2.071917
H        -3.875887   -1.504595   -0.576718
H        -4.812811   -0.033619   -1.004929
H        -3.355414   -0.498596   -1.921999
H         3.496888    1.632595   -0.105020

1b.tsZ.int.MeOLiMe
SCF Energy: -3235.08851701
C         1.612798    1.027885    0.358257
C         1.725755   -0.213794    1.256332
C         0.417520   -0.949139    0.943397
C        -0.602622    0.188520    0.885554
C         0.200101    1.211137    0.061884
C         3.010827   -1.023483    1.118689
Br        0.503696   -1.955627   -0.799211
C        -1.004734    0.663596    2.283889
O        -1.815294   -0.331741    0.226174
C        -2.913327    0.305783   -0.075306
C        -4.018602   -0.641726   -0.456236
O        -0.284739    1.944919   -0.842603
C         2.654165    1.666035   -0.222339
C         2.645086    2.630927   -1.368539
O        -3.080389    1.530866   -0.053670
H         1.639507    2.888802   -1.688845
H         3.184388    3.548142   -1.100298
H         3.178364    2.208290   -2.229565
H         2.921043   -1.950641    1.690167
H         3.209661   -1.284915    0.078801
H         3.870838   -0.471264    1.508803
H         1.654581    0.076554    2.314093
H        -0.148802    1.092444    2.804420
H        -1.357153   -0.196088    2.860003
H        -1.785011    1.427836    2.239213
H        -4.504835   -0.993978    0.458669
H        -4.760303   -0.130496   -1.067664
H        -3.616445   -1.512814   -0.971969
H         3.645494    1.425483    0.158689
Li       -1.893035    2.657596   -0.811612

2
SCF Energy: -3038.92945814
C        -4.870626   -0.534419   -1.015328
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C       -3.565962    0.239970   -0.965876
C       -2.699888    0.219740    0.020574
C       -1.601028    0.565610    0.740878
O       -1.495917    1.521385    1.568349
C       -0.342583   -0.423257    0.622551
C        0.813904    0.370310    0.032110
Br       2.462841   -0.717182   -0.374585
C        0.008610   -0.861119    2.058920
C       -0.657805   -1.656103   -0.240691
C        0.892981    1.678075   -0.176837
C        2.010474    2.506300   -0.728520
H       -5.006132   -1.114446   -0.098403
H       -4.905658   -1.230624   -1.867467
H       -5.738792    0.133089   -1.126859
H       -3.396564    0.856866   -1.866729
H        0.942653   -1.430769    2.098020
H        0.088550    0.025307    2.688345
H       -0.796419   -1.487788    2.456104
H        0.005697    2.211034    0.163563
H        2.400898    3.186597    0.039233
H        2.839940    1.904452   -1.099859
H        1.648725    3.139409   -1.547604
H        0.171373   -2.368818   -0.235045
H       -1.549669   -2.149464    0.148954
H       -0.865163   -1.375174   -1.275236

3.tsE
SCF Energy: -3038.90254012
C       -1.127643   -1.806031    1.558908
C       -0.489082   -0.451135    1.412750
C        0.702815   -0.174690    0.774659
C        0.862743    1.280380    0.367169
C       -0.482733    1.615784   -0.385378
O       -0.534642    2.621419   -1.111414
Br       1.297394   -1.538444   -0.549616
C        2.057725    1.606584   -0.533913
C        0.961975    2.190209    1.614990
C       -1.568339    0.744198   -0.058847
C       -2.482653    0.214142   -0.872221
C       -3.753422   -0.478461   -0.444649
H       -3.889499   -0.409392    0.638459
H       -4.636606   -0.027613   -0.923636
H       -3.769950   -1.544304   -0.718284
H       -2.107275   -1.720593    2.035398
H       -1.260077   -2.290406    0.591012
H       -0.504989   -2.465417    2.177106
H       -0.726544    0.234860    2.216579
H        2.054901    1.005000   -1.443045
H        3.004842    1.431167   -0.011795
H        1.997403    2.655015   -0.831267
H       -2.347841    0.275520   -1.963929
H        0.981871    3.235659    1.293034
H        0.108351    2.073192    2.284867
H        1.875435    1.975618    2.182562

3.tsZ
SCF Energy: -3038.90191091
C       -0.812209   -1.753953    2.003458
C       -0.260991   -0.400930    1.649229
C       -0.728397    0.456460    0.677931
C        0.287230    1.487265    0.215029
C        1.592065    0.643975   -0.076064
O        2.519748    1.178081   -0.714407
Br      -1.911491   -0.347975   -0.703312
C        0.602495    2.497058    1.344045
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C	−0.084952	2.295758	−1.032155
C	1.607941	−0.635640	0.540855
C	1.979596	−1.849217	0.132561
C	2.262847	−2.249361	−1.301924
H	2.325723	−1.365902	−1.940070
H	3.215840	−2.792694	−1.385500
H	1.488763	−2.914932	−1.712549
H	−1.789973	−1.666742	2.495017
H	−0.938775	−2.376201	1.117049
H	−0.134685	−2.271041	2.688264
H	0.247679	0.092463	2.468984
H	0.916734	2.004200	2.266023
H	−0.272864	3.118014	1.569592
H	1.424419	3.143958	1.023453
H	2.089641	−2.666325	0.858904
H	0.767229	2.918275	−1.310177
H	−0.313528	1.649048	−1.879906
H	−0.955758	2.933876	−0.845684