Supplementary Information

The Effect of Geminal Substitution on the Strain Energy of Dioxiranes. The Origin of the Low Ring Strain of Dimethyldioxirane.

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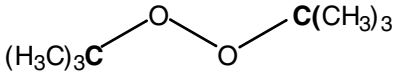
Table S1. Total energies calculated at the G2(MP2) and G2 level of theory (at 0 K). Total electronic energies calculated at B3LYP/6-311+G(3df,2p) and CBS-Q levels of theory are given in parentheses and in italic, respectively.

compound	G2MP2	G2
Hydrocarbons		
H•	-0.50000	-0.50000
H2	-1.16636	-1.16636
•CH_3	-39.74391	-39.74509
CH_4	-40.40966	-40.41088
•C_2H_5	-78.96812	-78.97034
C_2H_6	-79.62893	-79.63090
propane	-118.85308 (-119.1884)	-118.85580
$CH_3CH_2CH_2$• (C_1)	-118.19125	-118.19403
$CH_3CH_2CH_2$•	-118.19124	-118.19401
cyclopropane	-117.62885 (-117.93943)	-117.63115 *-117.63119*
n-butane (anti)	-158.07764	-158.08114
isobutane	-158.08081	-158.08431
methylcyclopropane	-156.85653	-156.85972
cyclobutane	-156.85542	-156.85860
n-pentane (anti)	-197.30223	-197.30657
cyclopentane	-196.11020	-196.11424
n-hexane (anti)	-236.52690 (-237.16839)	-236.53204
n-hexane (all-gauche)	-236.52489	
cyclohexane	-235.34420	-235.34902
2,2-dimethylpropane(neopentane)	-197.31051 (-197.84344)	-197.31478 *-197.31503*
1,1-dimethylcyclopropane	-196.08660 (-196.59818)	-196.09060
cis-1,2-dimethylcyclopropane	-196.08230	-196.08634
trans- 1,2-dimethylcyclopropane	-196.08443	-196.08849
1,1-dimethylcyclobutane	-235.31504	-235.31992
Ethers		
oxirane (ethylene oxide)	-153.52931	-153.53289
propylene oxide	-192.76153	-192.76604
E-2-butene oxide	-231.99408	-231.99949
Z-2-butene oxide	-231.99206	-231.99746
isobutylene oxide	-231.99620	-232.00024

dimethyl ether	-154.74283	-154.74668
CH_3OCH_2•	-154.08947	-154.09337
HCF_2OCH_3		*-353.11093*
diethyl ether (anti)	-233.20142	-233.20695
$CH_3CH_2OCH_3$	-193.97215	-193.97684
$CH_3CH_2OCH_2$•	-193.31879	-193.32353
ethyl propyl ether (anti)	-272.42567	
$CH_3CH_2OCH_2CH_2$•	-232.53806	-232.54369
$CH_3CH_2OCH_2CH_2CH_2$•	-271.76416	
$CH_3OCH_2OCH_3$ (Cs)	-269.09003	-269.09676
$CH_3OCH_2OCH_3$ (C2v)	-269.09881	-269.10563
$CH_3OCF_2OCH_3$ (Cs)	-467.44443	-467.45802 *-467.48454*
CH_3O-$C(CH_3)_2$-OCH_3 (Cs)	-347.55083	-347.55927
CH_3O-$C(CH_3)_2$-OCH_3 (C2v)	-347.56282	-347.57136
$CH_3OCH_2CH_2OCH_3$ (anti)	-308.31311	-308.32054
oxetane	-192.75571	-192.76007
tetrahydrofuran (THF)	-232.01052	-232.01572
tetrahydropyran (THP)	-271.24180	-271.24776
1,4-dioxane	-307.13700	-307.14418
1,3-dioxacyclopentane	-267.91330	-267.91977
1,3-dioxacyclohexane	-307.14556	*-307.16256*
2,2-dimethyl-1,3-dioxacyclohexane		*-385.62987*
2,2-difluoro-1,3-dioxacyclohexane		*-505.53333*
2,-trifluoromethyl-2-methyl-1,3-dioxacyclohexane		*-683.15351*
Thio ethers		
ethylene sulfide	-476.15703	-476.16447
thiacyclohexane	-593.85913	
Peroxides		
hydrogen peroxide	-151.35715	-151.36578
HOO•	-150.72278	-150.72792
methyl hydroperoxide	-190.57706	-190.58238
CH3OO•	-189.94087	-189.94375
dimethylperoxide (*anti*)	-229.79301	-229.79910
HCF_2OOCF_2H		*-626.51006*
CH_3OOCH_2•	-229.13685	-229.14304
ethyl hydroperoxide (Cs)	-229.80575	-229.81193
ethyl hydroperoxide (C_1)	-229.80633	-229.81251
isopropyl hydroperoxide	-269.03751	-269.04450
n-propyl hydroperoxide	-269.03038	-269.03734
$CH_3OOCH_2CH_3$	-269.02218	-269.02912
$CH_3OOCH_2CH_2CH_3$	-308.24629	-308.25401

CHF_2OOH	-388.90502	-388.91649
$CHF_2OO•$	-388.27217	-388.26003
diethyl peroxide	-308.25140 (-308.91574)	-308.25920
$CH_3CH_2OO•$	-229.17043	-229.17727
$HOOCH_2OOH$	-340.74366	-340.76073
ethylmethylperoxide	-269.02218	-269.02912
$CH_3\ CH_2OOCH_2•$	-268.43324	-268.44096
$CH_3OOCH_2CH_2•$	-268.35852	-268.36557
	(-466.23406)	*-465.20214*
dioxirane (DO)	-189.36718 (-189.6915)	-189.37220 *-189.38113*
methyldioxirane	-228.60471	-228.61073
dimethyldioxirane (DMDO)	-267.84190 (-268.36941)	-267.84877 *-267.85927*
difluorodioxirane (DFDO)	-387.70088	-387.71245 *-387.73971*
methyl(trifluoromethyl) dioxirane	-565.31741 (-566.19873)	*-565.37062*
1,2-dioxacyclobutane (dioxetane)	-228.57919	-228.58482
methyldioxetane	-267.81324	-267.81979
1,1-dimethyldioxetane	-307.04805	
1,2-dioxacyclopentane	-267.83679	-267.84329
1,2-dioxacyclohexane	-307.06678	-307.07357 *-307.16256*
1,2-4,5-tetraoxacyclohexane	-378.79682	
3,3-dimethyl-1,2,4,5-tetraoxacyclohexane		*-457.29798*
3,3-difluoro-1,2,4,5, -tetraoxacyclohexane		*-577.17740*
3,3-dimethyl-1,2-dioxacyclohexane	-385.53089	
3,3-difluoro-1,2-dioxacyclohexane	-505.40115	-505.41476
Amines		
methylamine	-95.66453	-95.66691
ethylamine	-134.89137	-134.89458
aziridine	-133.66135	-133.66414
oxazirdine	-169.52963	-169.53371
dimethylamine	-134.87958	-134.88280
CH_3NHCH_2	-134.23341	-134.23672
diethylamine	-213.33417	-213.33905
$C_2H_5NHCH_2CH_2$	-212.67219	-212.67715

$CH_3CH_2NHCH_3$	-174.10687	-174.11091
$C_2H_5NHCH_2$	-173.45900	-173.46312
azacyclobutane	-172.88800	-172.89168
ethylpropylamine (anti)	-252.55860	
piperidine	-251.37509	
pyrrolidine	-212.14288	-212.14743
2-oxapiperidine	-287.23076	

Fluorocarbons		
CF_4	-437.05269	
CH_2F_2	-238.71103	-238.71797
1,3-difluoropropane	-317.15210	
2,2-difluoropropane	-317.18422	-317.19297
1,1,1-trifluoropropane	-416.34741	
1,1,1-trifluoropentane	-494.79646	
2-methyl-2-trifluoromethyl-propane	-494.80460	
1-methyl(1-trifluoromethyl)cyclopropane	-493.57973	
1,1,1-trifluoropentane	-494.79646	
1,1-difluorocyclopropane	-315.93875	-315.94696
$C_2H_5CF_2OH$	-392.33213	
Alcohols		
methanol	-115.53181	-115.53489
ethanol	-154.76051	-154.76446
n-propanol	-193.98463	-193.98938
isopropanol	-193.99132	-193.99608
1,2-ethane diol	-229.89022	-229.89618
1,4-butane diol (anti)	-308.34066	
HO•	-75.64092	-75.64391
CH_3O•	-114.86465	-114.86869
$HOCH_2O$•	-114.87843	-114.88156
$HO(CH_3)_2O$•	-268.47399	-268.48182
$HO(CH_3)_2$•	-269.14589	-269.15297
CH_3OCH_2O•	-229.21886	-229.22579
CH_3CH_2O•	-154.09274	-154.09759
$CH_2(OH)_2$ (C_{2V})	-190.67832	-190.68360
$CH_2(OH)_2$ (Cs, first-order saddle point)	-190.66825	-190.67343
$(CH_3)_2C(OH)_2$ (C_{2V})	-269.14589	-269.15297
$(CH_3)_2C(OH)_2$	-269.14168	-269.14863
$(CH_3)_2C(OH)_2$ (Cs)	-269.13600	-269.14295
1,3-propane diol	-269.11476	-269.12157
CHF_2OH		-313.87900
$F_2C(OH)_2$ (Cs)	-389.02442	-389.03647
$F_2C(OH)2$ (one H-bond)	-389.02456	-389.03657

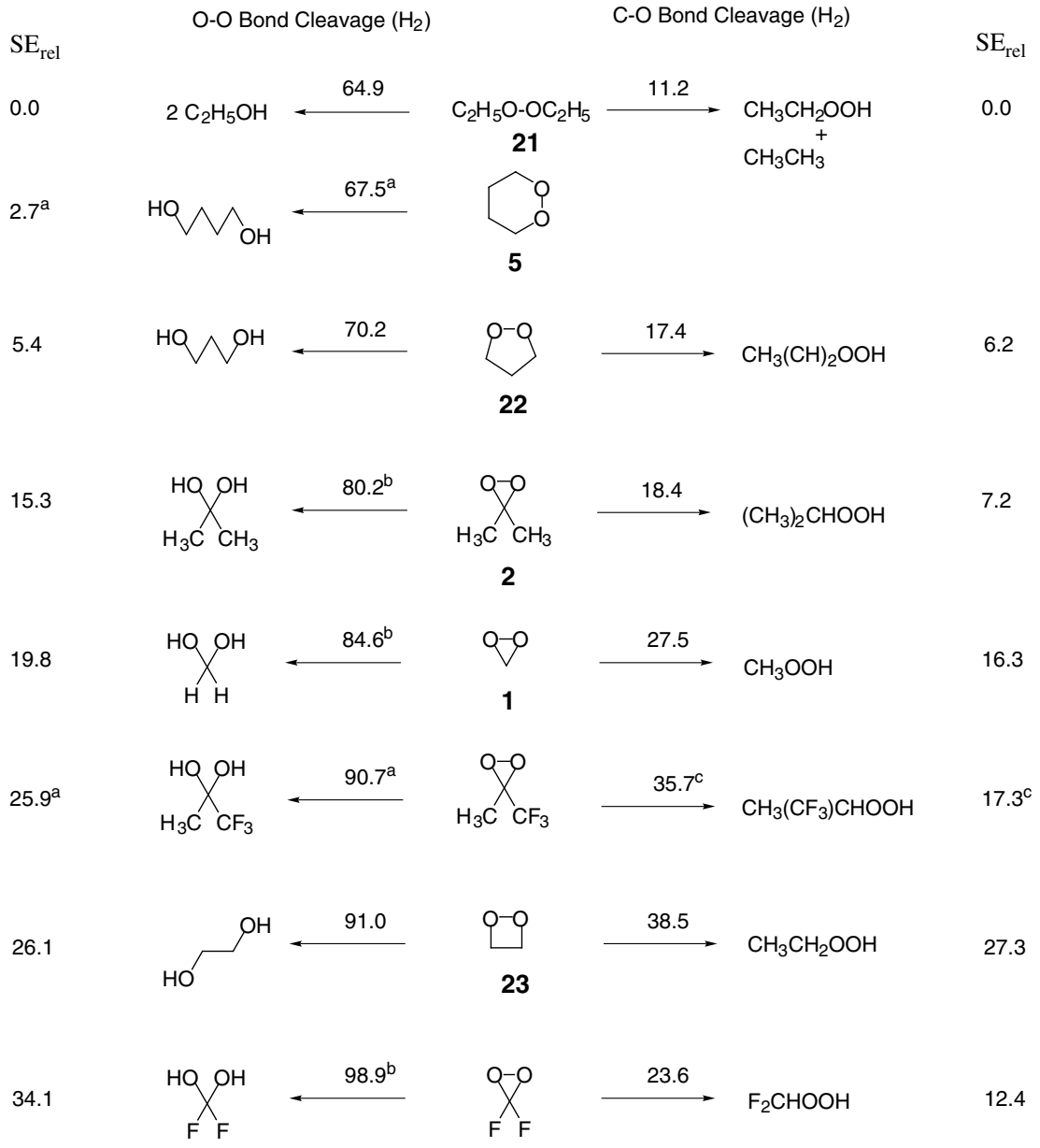
1,1-dihydroxycyclopropane (C_s)	-267.89789	
1,1-dihydroxycyclopropane (C_1)	-267.91703	
$CH_3(CF_3)C(OH_2)$	-566.62837	
Acids/Ester		
formic acid	-189.51126	-189.51648
methylacetate	-267.95828	-267.96526

Table 2S. CBS-APNO energies of the selected compounds and corresponding QCISD/6-311G(d,p) geometries.

compound	CBS-APNO (0 K)	CBS-APNO Enthalpy
cyclopropane C,0,-0.7553913947,-0.0000036779,0.4366975413 C,0,-0.0004954527,0.0000073249,-0.8725368631 C,0,0.7558868532,-0.0000036746,0.435839394 H,0,-1.2627044367,0.9134212032,0.7299874996 H,0,-1.262706417,-0.9134325432,0.7299714492 H,0,1.263534603,-0.9134325355,0.728536995 H,0,1.2635326303,0.9134212198,0.7285530139 H,0,-0.0008282075,-0.913415443,-1.4585311584 H,0,-0.0008282069,0.9134382641,-1.4585182327	-117.807484	-117.803163
DO O,0,0.750762982,-0.4353876783,0. C,0,0.,0.7272900849,0. O,0,-0.750762982,-0.4353876783,0. H,0,0.,1.3012311718,-0.9273384273 H,0,0.,1.3012311718,0.9273384273	-189.585841	-189.581888
DMDO C,0,-0.0483854932,0.,-0.0745928855 O,0,-0.0402445906,-0.0000000007,1.3178916664 O,0,1.2197976558,0.0000000007,0.5005514464 C,0,-0.4730664252,1.2909050809,-0.7292968885 C,0,-0.4730664232,-1.2909050809,-0.7292968897 H,0,-0.0928846852,2.1309374977,-0.1431945005 H,0,-0.092884682,-2.1309374977,-0.1431945026 H,0,-0.0750888459,1.3442458467,-1.7492786603 H,0,-1.5666837085,1.3442458451,-0.7817392966 H,0,-1.5666837065,-1.3442458467,-0.7817392979 H,0,-0.0750888439,-1.3442458451,-1.7492786616	-268.179663	-268.173115
1,2-dioxacyclopentane O,0,-0.9873033242,-0.2975426163,0.6558726893 O,0,-0.9872898048,0.2975615813,-0.6558845201 C,0,0.2645757795,-0.1417192214,-1.1776649587 C,0,1.2508649798,-0.0000131572,0.0000077933 C,0,0.2645640188,0.1417151725,1.1776678965 H,0,0.185964157,-1.1840535955,-1.509034575	-268.175531	-268.170057

H,0,0.4858417073,0.5113849937,-2.0255314236 H,0,1.8865570472,-0.8849178916,0.095353994 H,0,1.8865782944,0.8848771636,-0.0953303706 H,0,0.4858065221,-0.5113911429,2.025538842 H,0,0.1859686358,1.1840519896,1.509033793		
1,3-dioxacyclohexane O,0,-1.1703444811,-0.2785591937,0.7121774535 C,0,0.,0.1782213093,1.3355862668 O,0,1.1703444811,-0.2785591937,0.7121774535 C,0,1.2395295761,0.2114156449,-0.6216957261 C,0,0.,-0.2260477637,-1.4039880903 C,0,-1.2395295761,0.2114156449,-0.6216957261 H,0,0.,1.2851738386,1.352071048 H,0,0.,-0.2229163901,2.3490485339 H,0,1.3064188333,1.3132434758,-0.6077511839 H,0,2.1606437639,-0.1875504302,-1.0540424292 H,0,0.,0.2115724399,-2.4104735824 H,0,0.,-1.3182978926,-1.4911383763 H,0,-1.3064188333,1.3132434758,-0.6077511839 H,0,-2.1606437639,-0.1875504302,-1.0540424292	-307.542889	
22-dimethyl-1,3-dioxacyclohexane O,0,1.1748854507,-0.3780955867,-0.1131787571 C,0,0.0000000615,-0.0221102028,-0.8268634643 O,0,-1.1748853338,-0.3780958987,-0.1131789246 C,0,-1.2365300714,0.1362247401,1.2114029249 C,0,-0.0000000998,-0.2921222535,1.9977889291 C,0,1.2365298635,0.1362250734,1.2114030992 H,0,-1.3232882149,1.233951479,1.204375341 H,0,-2.1543318981,-0.2716557665,1.6439122889 H,0,-0.000000234,0.1568791079,2.9993052058 H,0,0.0000000345,-1.3837848288,2.0968336707 H,0,1.3232877118,1.2339518357,1.2043755232 H,0,2.1543317395,-0.2716551841,1.6439125937 C,0,0.0000002728,-0.8964524335,-2.0700056694 H,0,0.000000381,-1.9450582536,-1.7599498312 H,0,-0.8947072681,-0.6947609607,-2.667077519 H,0,0.8947078169,-0.6947607042,-2.6670774083 C,0,-0.0000001094,1.468019402,-1.1915462677 H,0,-0.8930076518,1.6938875143,-1.7834053719 H,0,-0.0000002772,2.1199439302,-0.3140151434 H,0,0.8930074821,1.6938877603,-1.783405206	-386.126308	-386.117339

Figure S1. Energies of Hydrogenation (ΔE, kcal/mol) of Cyclic Peroxides and Strain Energies (SErel., kcal/mol) Relative to the Acyclic Reference Compound, Diethyl Peroxide, at the G2 Level of Theory.



[a] G2(MP2); [b] the energy is calculated using the constrained Cs geometry of the diol reference compound; [c] B3LYP/6-311+G(3df,2p).

Appendix (coordinates)
HYDROCARBONS

cyclobutene
\G2MP2=-155.6407657\G2=-155.6438739
Charge = 0 Multiplicity = 1
C -0.7267807679,-0.0000426034,-0.7540121489
C -0.7323642334,0.0000447265,0.7578055761
C 0.6091754841,0.0000502149,0.8599604043
C 0.8325711766,-0.0000393119,-0.6352714867
H -1.1489455473,-0.889511698,-1.2332691217
H -1.1489400606,0.8893734468,-1.2333721484
H 1.3224397504,-0.8895064015,-1.0450791897
H 1.3224423736,0.8893787927,-1.0451828904
H -1.5397385598,0.0000992454,1.4849944109
H 1.2971320877,0.0000884585,1.7010148709

cyclobutane radical
\G2MP2=-156.1955646\G2=-156.1989294\
Charge = 0 Multiplicity = 2
C 0.8173641927,-0.09347373,-0.7276754435
C 0.6941700747,0.0887931679,0.8106370431
C -0.8447785857,-0.0934733111,0.6956619558
C -0.6786070118,0.0142382923,-0.7924624683
H 1.403500709,0.658407906,-1.2691376457
H 1.2045832519,-1.0818091586,-1.0134005361
H 0.9715140778,1.0943187958,1.1345131043
H 1.2249018791,-0.6379767342,1.4304144344
H -1.4699818211,0.6584086301,1.1915024417
H -1.1866831316,-1.0818085559,1.0343049434
H -1.377777635,-0.1339613024,-1.6089388292

2-methylbutane
\G2MP2=-197.3046195\G2=-197.3089557
Charge = 0 Multiplicity = 1
C 0.2882641635,-0.0645287935,-1.0053565301
C 0.2634940539,0.0051317006,0.5229805086
H 1.3343663637,-0.0985389666,-1.3347301536
H -0.1287299445,0.8696489551,-1.4054872933
C 1.1436849553,1.1504706328,1.0163303761
H 0.6824245701,-0.9366808014,0.906235154
H 1.1691689932,1.189089306,2.1097291096
H 2.1719700503,1.044323671,0.6571046071
H 0.7586063175,2.1105490278,0.6557211699
C -1.1537729685,0.1521231865,1.0702220023
H -1.1423468886,0.2335064673,2.161510905

H -1.622745097,1.0589449058,0.6718389305
H -1.7871632245,-0.698974224,0.8083705009
C -0.4576272581,-1.2557213556,-1.5985926311
H -0.3246303664,-1.298432891,-2.6833615476
H -0.0843859382,-2.1954306673,-1.1793359794
H -1.5307925117,-1.2028570073,-1.4010977574

1,1-dimethylcyclobutane
Charge = 0 Multiplicity = 1 G2MP2=-235.31504 a.u.
C -0.2895890802,0.0760876907,-1.2615393374
C -0.2699373665,0.1231081051,0.2883953518
C 1.2779109627,0.0760731905,0.2056431709
C 1.1545697234,-0.4668362044,-1.2335171931
H -1.0648564484,-0.5340585915,-1.7375952777
H -0.3281185061,1.0851152665,-1.6861996954
H 1.8041216796,-0.5340851315,0.9477727685
H 1.7041987309,1.0850964662,0.216052437
H 1.1832958924,-1.5590288749,-1.26421826
H 1.8544261114,-0.0840374264,-1.9812219806
C -0.8832001078,1.3463246087,0.9436015469
H -1.9706853471,1.3590083406,0.8088432602
H -0.6769163199,1.3589963748,2.0198131029
H -0.4771230877,2.2657038355,0.5097684109
C -0.8358832467,-1.1547570248,0.8930247506
H -0.6271264888,-1.1979754857,1.9676022426
H -1.9219018949,-1.1979635113,0.7556904322
H -0.4025396561,-2.0467734569,0.4300427966

cycpentane
\G2MP2=-196.1102018\G2=-196.1142422
Charge = 0 Multiplicity = 1
C -0.3659970667,-0.1495907392,-1.2251456435
C 1.0210766864,0.2571833405,-0.718802413
C 1.0210485405,-0.2571835204,0.7188413229
C -0.3660427454,0.1495968243,1.2251305214
C -1.2986212956,-0.0000057632,-0.000023249
H -0.697798783,0.4426854971,-2.0830711569
H -0.337741885,-1.1953420475,-1.5501382155
H 1.1185511399,1.3496827281,-0.7165012443
H 1.8350065373,-0.1457626878,-1.3296066973
H 1.1185176066,-1.3496833695,0.7165458214
H 1.8349572326,0.1457605949,1.3296750385
H -0.6978765662,-0.442667084,2.0830522054
H -0.3377987107,1.1953530833,1.5501081023
H -1.9522915179,-0.8712695915,0.1015619223
H -1.9523097684,0.8712420251,-0.1016290089

2,2-dimethylepropane (neopentane)
\G2MP2=-197.3105102\G2=-197.3147783\
Charge = 0 Multiplicity = 1
C -0.5494353188,1.4191377913,0.1409795978
C 0.0000000326,-0.0000000277,0.000000009
H 0.1720128099,2.0696988419,0.6457240038
H -0.7672381963,1.8536478541,-0.8399622477
H -1.4750923886,1.4240824406,0.7254610222
C -1.0318226731,-0.8778244674,-0.7074409599
H -0.6620696968,-1.9019375462,-0.8212791449
H -1.966879678,-0.9176747658,-0.1394934736
H -1.2590443307,-0.4881031335,-1.7049235885
C 1.2894023921,0.0320291376,-0.8198305953
H 1.7044183002,-0.974343232,-0.9358497691
H 1.1074483834,0.4394837976,-1.8195092646
H 2.046708687,0.6555477004,-0.3338308299
C 0.2918555705,-0.573342431,1.3862919488
H 0.6874320469,-1.5915140662,1.3132866681
H 1.0296997287,0.0383766267,1.9153191623
H -0.6173956852,-0.6072645351,1.9950574595

2,2-dimethylbutane
\G2MP2=-236.5333856\G2=-236.5385078\
Charge = 0 Multiplicity = 1
C 0.0853115193,0.4572543025,-1.5430725459
C -0.0078648786,0.4315936596,-0.0174594229
H 1.1271896013,0.377088728,-1.8723610168
H -0.4791751352,-0.361558821,-1.9979787888
H -0.3200431908,1.3962011406,-1.9349227485
C -1.474893922,0.5076457981,0.4054799676
H -1.5699356041,0.4641882831,1.4960971334
H -1.9221885333,1.4479524593,0.06602288
H -2.0628869532,-0.3104017272,-0.0200811901
C 0.6587544049,-0.8325651487,0.5489965174
H 0.6252350963,-0.7720123587,1.6451215889
H 1.722101217,-0.8074398609,0.2752400347
C 0.731280036,1.647645206,0.5429245565
H 0.680109442,1.6665727419,1.636872758
H 1.7875892632,1.6307978064,0.2537425497
H 0.292824721,2.5785500243,0.1677729131
C 0.0669554199,-2.1691388632,0.1097090444
H 0.1251964325,-2.3028204349,-0.9732825942
H 0.6167379541,-2.9946014765,0.571264193
H -0.9800097878,-2.2671262305,0.4070235849

2-methylbutane
\G2MP2=-197.3046195\G2=-197.3089557
Charge = 0 Multiplicity = 1
C 0.2882641635,-0.0645287935,-1.0053565301
C 0.2634940539,0.0051317006,0.5229805086
H 1.3343663637,-0.0985389666,-1.3347301536
H -0.1287299445,0.8696489551,-1.4054872933
C 1.1436849553,1.1504706328,1.0163303761
H 0.6824245701,-0.9366808014,0.906235154
H 1.1691689932,1.189089306,2.1097291096
H 2.1719700503,1.044323671,0.6571046071
H 0.7586063175,2.1105490278,0.6557211699
C -1.1537729685,0.1521231865,1.0702220023
H -1.1423468886,0.2335064673,2.161510905
H -1.622745097,1.0589449058,0.6718389305
H -1.7871632245,-0.698974224,0.8083705009
C -0.4576272581,-1.2557213556,-1.5985926311
H -0.3246303664,-1.298432891,-2.6833615476
H -0.0843859382,-2.1954306673,-1.1793359794
H -1.5307925117,-1.2028570073,-1.4010977574

dimethylcyclopropane
G2MP2=-196.08660/G2=-196.09060
Charge = 0 Multiplicity = 1
C 0.0587204562,0.0221323987,-1.3732562924
C -0.0876724176,-0.0000262235,0.121961725
C 1.2829934806,-0.0217383667,-0.4931814147
H -0.2026958862,-0.8743396534,-1.9273570666
H -0.1598179674,0.9483313547,-1.8961564762
H 1.8913292602,0.8748341687,-0.421672563
H 1.8484553534,-0.9478363707,-0.4528879446
C -0.5940725072,-1.269065206,0.763143042
H -0.2507948301,-1.3455892408,1.8007178197
H -1.6893448043,-1.2940408805,0.7665866992
H -0.2380511535,-2.1520149607,0.2238796057
C -0.5343602193,1.2687342906,0.8066021678
H -1.6272489265,1.3450538576,0.8117695951
H -0.1887101397,1.2934766872,1.8459147877
H -0.1367736626,2.1519036792,0.2975901765

2-methylpentane G2MP2=-236.52927\G2=-236.5344095\
Charge = 0 Multiplicity = 1
C -0.6413433162,-0.0299002007,-2.2909998848
C 0.1333860233,-0.4133885256,-1.0327254931
H -1.691130856,-0.3303651924,-2.2179717657
H -0.6112742422,1.0546991954,-2.441972922

H -0.2141393686,-0.5040725271,-3.1801019956
C 1.6019306559,-0.0218784943,-1.1748933961
H 0.0796312862,-1.5058566072,-0.9193087122
H 2.2036137528,-0.3653716107,-0.3298710726
H 2.032114788,-0.4513336962,-2.0850679951
H 1.6999134661,1.0676864792,-1.2401655567
C -0.51550985,0.2146268774,0.2024517535
H -0.4693119818,1.3093732269,0.1082716927
H -1.5827268603,-0.0465167004,0.2083065462
C 0.0936024758,-0.2027166335,1.5379120916
H 1.134674637,0.1316854812,1.5966822208
H 0.1155996211,-1.2983473718,1.59650275
C -0.6804537562,0.3575611347,2.7268392993
H -1.7163668013,0.0055255805,2.7191091319
H -0.2301124537,0.0558973434,3.6767940154
H -0.7001583826,1.4511714504,2.6972874407

n-hexane all trans conformation
G2MP2=-236.52690/G2=-236.53204
Charge = 0 Multiplicity = 1
C -0.0071177685,0.0132939256,-0.7624192889
C 0.0071717363,-0.0132625758,0.7624195047
H 1.0253336385,-0.0163148292,-1.1357120664
H -0.4951065491,-0.8965855735,-1.1368055492
C 0.7144241982,-1.2357923488,1.3383720751
H 0.4952436997,0.8965781875,1.136792967
H -1.0252717627,0.0164373491,1.1357253516
C 0.7219475476,-1.2506896395,2.8630424819
H 0.2261406313,-2.1436617521,0.9633935923
H 1.7452761645,-1.264300428,0.964488219
H 1.2335975269,-2.1350325167,3.25327428
H 1.2308991929,-0.3665980701,3.2585811493
H -0.2986018867,-1.2520022276,3.2574758022
C -0.7144668327,1.2357677671,-1.3383721281
H -1.7453292949,1.2641783859,-0.9645109695
H -0.226273245,2.1436767891,-0.963371342
C -0.7219592211,1.2506826812,-2.8630426328
H 0.2985982406,1.2520797659,-3.2574547325
H -1.2308336037,0.3665560463,-3.2586024342
H -1.2336707109,2.1349900143,-3.2532743389

n-hexane all gauche
G2MP2=-236.52489
Charge = 0 Multiplicity = 1
C 1.0122134638,-0.0297255094,-2.4318825755
C 1.5916170308,0.5074860066,-1.1268100168

H 1.7625214195,-0.0214289516,-3.2276219472
H 0.6574737181,-1.0574773391,-2.3234996274
H 0.1676586562,0.5835850319,-2.7619952199
C 0.5653147557,0.6208226102,0.0003520995
H 2.4162421187,-0.1376220255,-0.7984683427
H 2.0292640638,1.4962024691,-1.3093139129
C -0.0259953075,-0.7191863207,0.4325465063
H 1.0416048579,1.0919606653,0.8707210484
H -0.2356639592,1.2990774999,-0.318184296
H -0.6322629333,-1.1407794815,-0.3784780219
H 0.7960168943,-1.4271163181,0.604291969
C -0.8827306576,-0.6367758516,1.695815746
H -1.1882455262,-1.6495909986,1.9843793869
H -0.2697431241,-0.2538654771,2.5214095131
C -2.1261906487,0.2328977112,1.5377203613
H -2.7452662117,0.2006673191,2.4387967604
H -1.8671822703,1.278109287,1.3524950433
H -2.737789523,-0.114833558,0.6990149223

cyclohexane chair
G2MP2=-235.34420/G2=-235.34902
Charge = 0 Multiplicity = 1
C -1.1280315751,-0.5856722099,-0.7691232135
C -1.1246784742,-0.593563406,0.7676589614
C 0.3054331109,-0.5848215041,1.3309446272
C 1.1276745778,0.5859405608,0.7693424544
C 1.1247768957,0.5937200668,-0.7674285677
C -0.3051340754,0.5843857333,-1.3312904181
H 0.2803217293,-0.538681367,2.4273922133
H -1.6624384346,0.2936720627,1.134509006
H -1.6744169388,-1.4664149812,1.1429794985
H -0.7058032209,-1.533344964,-1.1360943839
H -2.1583073847,-0.539183391,-1.1450388381
H 0.7043600752,1.533206621,1.1361173299
H 2.1578262373,0.5403790319,1.145694431
H 1.674240187,1.4667877574,-1.1426535096
H 1.6630797426,-0.2932902056,-1.1340255055
H -0.8014826217,1.5319262213,-1.0728174193
H -0.2793696265,0.5369865427,-2.4276763094
H 0.8017474976,-1.5319787737,1.0709904248

ETHERS
oxirane G2MP2=-153.5293084\G2=-153.5328901
Charge = 0 Multiplicity = 1
C -0.3734726318,0.,-0.7327545398
C -0.37762329,0.,0.7306302672

O 0.8608306006,0.,0.0024336371
H -0.5914665846,-0.9196719288,-1.2704455396
H -0.5914665846,0.9196719288,-1.2704455396
H -0.5985680525,-0.9196894833,1.267083809
H -0.5985680525,0.9196894833,1.267083809

propylene oxide G2MP2=-192.7615312\G2=-192.7660374
Charge = 0 Multiplicity = 1
C -1.0149935866,-0.3506268098,-0.5528537969
O -0.7328050139,-0.3057503599,0.8593788484
C 0.3669371022,-0.3578465397,-0.069827426
H -1.4756911793,-1.271191251,-0.9046957269
H -1.4268919099,0.5662896617,-0.9699956986
C 1.2339385368,0.8647113122,-0.1292370385
H 0.889940387,-1.3150802843,-0.0652554668
H 1.8915697035,0.9099426449,0.7428594427
H 1.8563755632,0.8561493698,-1.0290801485
H 0.6118452323,1.762464962,-0.1373536199

isobutene oxide G2MP2=-231.99620\G2=-232.00024
Charge = 0 Multiplicity = 1
C -1.04048 0.01434 -0.88531
O -1.18185 -0.06596 0.54927
C 0.14447 0.00572 -0.02279
H -1.32022 -0.88665 -1.42847
H -1.37752 0.94839 -1.33141
C 0.86922 1.29423 0.25953
C 0.94891 -1.25777 0.12455
H 1.26565 1.28686 1.27932
H 1.70683 1.42912 -0.43199
H 0.18776 2.14183 0.16123
H 1.34747 -1.33327 1.14073
H 0.32118 -2.13104 -0.06476
H 1.79101 -1.26666 -0.57457

dimethyl ether G2MP2=-154.7428253\G2=-154.7466746
Charge = 0 Multiplicity = 1
O 0.005750225,-0.5671964001,-0.1960773528
C -1.1647603357,0.2040653143,-0.0124775017
H -2.0084215431,-0.4276259784,-0.291606144
H -1.2793450094,0.5188552316,1.0343257982
H -1.1592310132,1.1014167175,-0.6471028394
C 1.1609290717,0.1738539354,0.1431227733
H 2.0176262314,-0.4799470387,-0.0221808025
H 1.2632167659,1.0699139584,-0.4850756529
H 1.1431403524,0.4874428119,1.1963868333

diethyl ether (anti) G2MP2=-233.20142\G2=-233.20695
Charge = 0 Multiplicity = 1

O	0.,-0.268557,0.
C	-1.17708,0.524555,0.
C	-2.363802,-0.412947,0.
H	-1.193525,1.177388,-0.886841
H	-1.193525,1.177388,0.886841
H	-3.300676,0.150909,-0.000003
H	-2.337933,-1.050553,-0.885809
H	-2.337936,-1.05055,0.885812
C	1.17708,0.524555,0.
C	2.363802,-0.412947,0.
H	1.193525,1.177388,0.886841
H	1.193525,1.177388,-0.886841
H	3.300676,0.150909,0.000003
H	2.337933,-1.050553,0.885809
H	2.337936,-1.05055,-0.885812

$CH_3CH_2OCH_3$ G2MP2(0 K)= -193.972148/ G2(0 K)= -193.976836
Charge = 0 Multiplicity = 1

O	-0.3296504639,0.5709722585,0.2708663024
C	-0.3229643127,0.5593910139,1.6853036726
H	0.7013406964,0.5686605327,2.0832560648
H	-0.8431459341,-0.3230476564,2.0832557621
C	0.3276393034,-0.5674888232,-0.2623327309
C	0.2706055324,-0.4687027597,-1.770110872
H	-0.1650681858,-1.4878580015,0.0891292145
H	1.3710559914,-0.6009778427,0.0891295011
H	0.7662600836,-1.3272028425,-2.231437032
H	-0.7681013775,-0.441321274,-2.1049546986
H	0.7662472812,0.4445339246,-2.1049543966
H	-0.843067991,1.4602385008,2.012484748

ethylpropylether G2MP2=-272.42567
Charge = 0 Multiplicity =1

8	-0.05539	0.00058	-0.70529
6	-0.06742	-0.00062	0.7131
6	1.36712	0.00103	1.19865
1	-0.60316	0.88584	1.09136
1	-0.60064	-0.88922	1.0899
6	1.45801	-0.00016	2.72059
1	1.87192	-0.87712	0.78399
1	1.8694	0.88133	0.78551
1	2.49924	0.00112	3.05239
1	0.97142	0.88296	3.14523

1	0.97407	-0.88548	3.14369
6	-1.36647	-0.00104	-1.24963
1	-1.91843	-0.88907	-0.90377
1	-1.92125	0.88465	-0.90227
6	-1.2391	0.00044	-2.75659
1	-0.69441	0.88741	-3.08595
1	-0.69159	-0.88422	-3.08746
1	-2.22622	-0.00073	-3.22702

methyl isopropyl ether G2MP2=-233.20167\G2=-233.20718
Charge = 0 Multiplicity = 1

O	0.273686277,0.3431138053,-0.8719305433
C	-0.1014417542,1.391540464,1.1928091264
C	0.1044463763,0.0509414951,0.516064866
H	0.7478024125,2.0483349649,0.9938805363
H	-1.0046821101,1.865642572,0.8000751559
H	-0.2106087853,1.2690857291,2.2738882155
C	-1.0654388308,-0.8931706331,0.7537268133
H	1.0304864104,-0.4129511468,0.8955697071
H	-0.9071806447,-1.8673990655,0.2853660487
H	-1.2123894717,-1.0584219385,1.8250942388
H	-1.9762866825,-0.4529841637,0.3388587101
C	0.8081952926,-0.7348598071,-1.618971005
H	1.7417537996,-1.1048886106,-1.1726754556
H	0.1075051207,-1.5733558589,-1.7109883361
H	1.0195432323,-0.344682038,-2.6154032781

$CH_3OCH_2OCH_3$ (anti) G2MP2=-269.0900269\G2=-269.0967559
Charge = 0 Multiplicity = 1

C	0.0000000462,0.0000234761,0.308741011
H	0.8975923049,0.000073464,0.9592161588
O	-0.0000000803,1.1119224286,-0.5365718207
O	-0.0000000802,-1.1120033895,-0.5364020468
H	-0.8975920179,0.000073464,0.9592164273
C	0.000000031,-2.3184113822,0.2073908126
H	0.892701307,-2.4016088188,0.8419724215
H	-0.8927010551,-2.4016088188,0.8419726886
H	-0.0000000778,-3.1289218006,-0.5201706392
C	0.000000031,2.3184423222,0.2070377894
H	-0.8927011866,2.4017358881,0.8416067131
H	0.8927014384,2.4017358881,0.8416064461
H	-0.0000000779,3.128841924,-0.5206469548

CH_3O $CH_2CH_2OCH_3$ (anti) G2MP2-308.31311\G2=-308.32054
Charge = 0 Multiplicity = 1

O	-0.681788,0.001049,-1.654401
C	-0.717149,-0.000754,-0.238704
C	0.717149,0.000936,0.238704
H	-1.239081,0.887209,0.147243
H	-1.236258,-0.891318,0.145053
O	0.681788,-0.000894,1.6544
H	1.23909,-0.887013,-0.147264
H	1.236249,0.891514,-0.145033
C	1.986017,0.000427,2.205253
H	2.548146,0.893628,1.900974
H	1.871263,-0.001115,3.289516
H	2.550902,-0.890264,1.898729
C	-1.986017,-0.000456,-2.205253
H	-2.548029,-0.893722,-1.900952
H	-2.551018,0.89017,-1.898752
H	-1.871263,0.001074,-3.289516

oxetane G2MP2=-192.7557131\G2=-192.7600707
Charge = 0 Multiplicity = 1

O	-0.7609205308,0.0002612219,-0.7608726826
C	-0.7739804509,0.0000826291,0.6886586716
C	0.7586837718,-0.0000016317,0.7586360044
C	0.6886099287,-0.0002853382,-0.7740237969
H	-1.2690400226,-0.8922436717,1.0873140172
H	-1.2690462385,0.8922973063,1.0875440188
H	1.2054326058,-0.889523491,1.2055806644
H	1.2054403948,0.8897379278,1.2051406301
H	1.0870096854,-0.8928363125,-1.2688840585
H	1.0876883242,0.8917045098,-1.2693390856

2,2-dimethyloxetane G2MP2=-271.22348/ G2=-271.22953
Charge = 0 Multiplicity = 1

C	-0.7838757546,0.2439195255,-1.483865508
O	-1.2022918127,0.1362559018,-0.1003290027
C	0.1843708038,-0.055683617,0.3337099063
C	0.6905613605,0.0507137096,-1.1179878617
H	-1.2278213258,-0.5441200682,-2.1022559587
H	-1.0445885364,1.2192286175,-1.909653542
H	1.1579490852,-0.8556640596,-1.5098004417
H	1.3407770039,0.9057933771,-1.3168515318
C	0.3396749817,-1.4157563569,0.9783978773
H	1.3862264975,-1.6059016551,1.2386238297
H	-0.26315808,-1.4671110308,1.8897212407
H	-0.0021108963,-2.197531719,0.2952365899
C	0.5988362644,1.0737789592,1.2513433933
H	-0.0011580065,1.0502210711,2.1656773472

H	1.6560894169,0.9865764563,1.5229208883
H	0.4387234084,2.036628474,0.759426757

THF G2MP2=-232.0105197\G2=-232.0157216
Charge = 0 Multiplicity = 1

C	-0.963111393,0.187751844,-0.7644260246
C	-1.0077278806,-0.1541463662,0.7194929185
C	0.3985096558,0.2448673429,1.1567952471
C	1.2225696538,-0.2264445568,-0.0347046076
O	0.385893926,-0.0573910645,-1.1884195503
H	-1.6333905863,-0.4241190854,-1.3757029641
H	-1.210613865,1.2450388335,-0.9318917601
H	-1.1551270687,-1.2300648713,0.8580118245
H	-1.8022756679,0.3734668446,1.2538659266
H	0.4671704821,1.332517247,1.260803991
H	0.7135974052,-0.2113255815,2.0990502969
H	2.1410299378,0.3483609264,-0.1874971628
H	1.4910177382,-1.2869153812,0.0677710496

THP G2MP2=-271.2417979/G2=-271.24776
Charge = 0 Multiplicity = 1

C	-1.0563412982,-0.5677257236,-0.752064767
C	-1.0605120725,-0.6140885246,0.768495127
C	0.3721000647,-0.5579699875,1.2949727281
C	1.1014780176,0.6382368907,0.6868589244
C	0.9733445609,0.6079629242,-0.8287051962
H	0.3839061143,-0.5070271962,2.3891136968
H	-1.626458176,0.2476766798,1.1402887688
H	-1.5734636972,-1.5199391654,1.1135998002
H	-2.070249595,-0.5220940848,-1.1581027246
H	0.6564193457,1.5700257269,1.0540878922
H	2.1603004923,0.6428310549,0.9726137997
H	1.4137055546,1.4959751213,-1.2896559926
H	1.4876250007,-0.2802174527,-1.2330565368
H	0.8963395969,-1.4813159725,1.0141050589
O	-0.3929913573,0.5980698863,-1.2330962484
H	-0.564609413,-1.4689672773,-1.1555646732

1,4-dioxane G2MP2=-307.13700/G2=-307.14418
Charge = 0 Multiplicity = 1

O	0.05174,0.01756,0.02994
C	0.03461,0.05112,1.45571
C	1.45035,0.03688,1.99493
O	2.17659,1.15917,1.49768
C	2.19372,1.12562,0.07192
C	0.77798,1.13985,-0.4673

H 1.46489,0.1165,3.08554
H -0.4826,0.9568,1.80667
H -0.52688,-0.82955,1.77996
H 2.75521,2.00628,-0.25233
H 2.71093,0.21994,-0.27905
H 0.28083,2.07491,-0.16823
H 0.76344,1.06023,-1.55791
H 1.94749,-0.89818,1.69586

PEROXIDES

methyl hydroperoxide G2MP2=-190.5770639\G2=-190.58237
Charge = 0 Multiplicity = 1
O 0.4509488141,0.0078069097,0.4295430166
C -0.7916685948,0.6951968781,0.4530890752
H -0.8597939894,1.4062878957,-0.3742471472
H -1.6330286511,-0.0030429364,0.4142460041
H -0.7854443381,1.2285476287,1.4059545926
O 0.4759120525,-0.6610577894,-0.8789901941
H 0.6133916144,-1.576966819,-0.5689104809

dimethylperoxide (*anti*) G2MP2=-229.79301\G2=-229.79910
Charge = 0 Multiplicity = 1
O 0.0315969185,0.,-0.7378898706
O -0.0315969185,0.,0.7378898706
C 1.3348798925,0.,1.1191416314
H 1.8434285326,-0.8959232983,0.751677264
H 1.8434285326,0.8959232983,0.751677264
H 1.3113686158,0.,2.2104666529
C -1.3348798925,0.,-1.1191416314
H -1.8434285326,-0.8959232983,-0.751677264
H -1.8434285326,0.8959232983,-0.751677264
H -1.3113686158,0.,-2.2104666529

ethyl hydroperoxide (Cs) G2MP2=-229.80575\G2=-229.81193
Charge = 0 Multiplicity = 1
O -1.3866957603,0.,1.152990258
H -1.2281047966,0.,2.1169514783
O 0.0303533607,0.,0.7300739108
C -0.0474664053,0.,-0.6907799706
H -0.5915702801,-0.8899948444,-1.0260723804
H -0.5915702801,0.8899948444,-1.0260723804
C 1.3861162342,0.,-1.1783399361
H 1.9121775874,0.887511314,-0.8217801951
H 1.9121775874,-0.887511314,-0.8217801951
H 1.4057304047,0.,-2.2710402375

ethyl hydroperoxide (C_1) G2MP2=-229.80633\G2=-229.81251
Charge = 0 Multiplicity = 1

O	-1.1791275655,-0.8305841608,1.104211991
H	-0.990260458,-1.7889633228,1.1043358532
O	-0.5304964468,-0.4804996032,-0.1674231063
C	0.4896903194,0.4552467339,0.1775391061
H	1.2237449159,-0.0206555169,0.8388001538
H	0.0429460572,1.3028648281,0.7077370301
C	1.1100644143,0.8817728157,-1.1366001057
H	1.907092445,1.6067029538,-0.9530972317
H	1.535908336,0.0223652952,-1.6582354214
H	0.3590323999,1.3442385768,-1.7794854645

isopropyl hydroperoxide G2MP2=-269.03751/G2=-269.04450
Charge = 0 Multiplicity = 1

C	0.1200019436,-0.3568298548,-1.7872707824
C	0.3108810415,-0.32393223,-0.2823672723
H	1.3748464881,-0.4208350446,-0.0328414897
H	0.7034938895,0.4322701102,-2.2654965563
H	0.4420273208,-1.3233296257,-2.1832905089
H	-0.9346987253,-0.2138565115,-2.0365432253
C	-0.4968630099,-1.3818344198,0.4446368222
H	-0.3627807657,-1.2893901613,1.5235447883
H	-1.5580428393,-1.2675300636,0.2048779045
H	-0.1778455913,-2.3836750773,0.1430537984
O	-0.1091893303,0.9995787204,0.081689245
O	0.2959668962,1.1859291969,1.4842960345
H	-0.5853401552,1.3578620626,1.8688204477

n-propyl hydroperoxide G2MP2=-269.0303816\G2=-269.0373346
Charge = 0 Multiplicity = 1

O	0.1325540429,0.3004658194,-1.2715201176
C	0.1583955805,0.2728725095,0.1535601885
H	1.1972505352,0.2887878388,0.5034756868
H	-0.3569288402,1.1546708279,0.5564762803
O	0.8822489785,1.5080540946,-1.6490005833
H	0.1680851306,1.9804007736,-2.1192145719
C	-0.5401547441,-1.0103825257,0.5611555703
H	-1.5555675178,-1.006643556,0.1524300018
H	-0.0138034306,-1.8550828732,0.1066212949
C	-0.5815572808,-1.1647785001,2.0784423679
H	0.427757018,-1.1888690284,2.4987570503
H	-1.1208925536,-0.3353498272,2.5446327106
H	-1.084425847,-2.0923423699,2.3620383952

diethyl peroxide G2MP2=-308.25140\G2=-308.25920
Charge = 0 Multiplicity = 1
O 0.0187244148,0.,-0.7397779081
O -0.0187244148,0.,0.7397779081
C 1.3561039155,0.,1.1108511407
C -1.3561039155,0.,-1.1108511407
H 1.8458161207,0.8906931787,0.7004268325
H 1.8458161207,-0.8906931787,0.7004268325
H -1.8458161207,0.8906931787,-0.7004268325
H -1.8458161207,-0.8906931787,-0.7004268325
C -1.3707745786,0.,-2.6254303854
H -0.8652957795,0.8864725337,-3.0130457055
H -0.8652957795,-0.8864725337,-3.0130457055
H -2.4022570702,0.,-2.9870143179
C 1.3707745786,0.,2.6254303854
H 0.8652957795,0.8864725337,3.0130457055
H 0.8652957795,-0.8864725337,3.0130457055
H 2.4022570702,0.,2.9870143179

ethylmethylperoxide G2MP2=-269.0221748\G2=-269.0291201
Charge = 0 Multiplicity = 1
O -0.2787933507,0.,-1.2710796992
O -0.2742214475,0.,0.2073593852
C 1.1104534713,0.,0.541000031
C -1.6616422625,0.,-1.5874262147
H 1.5892545857,0.8900126372,0.116970828
H 1.5892545857,-0.8900126372,0.116970828
H -2.1527015537,0.8958440924,-1.1964753384
H -2.1527015537,-0.8958440924,-1.1964753384
C 1.1660598517,0.,2.0545140581
H 0.672351449,0.8872308865,2.4555288983
H 0.672351449,-0.8872308865,2.4555288983
H 2.2069501183,0.,2.3879659226
H -1.6898670583,0.,-2.678779433

Dioxirane G2MP2=-189.3671767\G2=-189.3721962
Charge = 0 Multiplicity = 1
O -0.4376121288,0.,-0.765184826
C 0.7317298799,0.,0.
O -0.4376121288,0.,0.765184826
H 1.3057073904,0.9268325146,0.
H 1.3057073904,-0.9268325146,0.

methyldioxirane G2MP2=-228.6047061\G2=-228.6107246
Charge = 0 Multiplicity = 1
O -0.2608281064,0.3434515606,-1.1192069068

C -0.1275450673,0.3629416987,0.2758026782
O 1.0938301659,0.2773560309,-0.406355607
C -0.582470864,-0.8429803169,1.0289264044
H -0.0966999676,-0.8839243124,2.0079019369
H -1.6646800524,-0.8078030309,1.182665834
H -0.3227087414,-1.7320000136,0.453317474
H -0.319832127,1.3374983338,0.7322403703

dimethyldioxirane G2MP2= -267.841897\G2=-267.84877
Charge = 0 Multiplicity = 1
C 0.0962589558,0.,0.
O -1.08382712,0.,-0.7662802131
O -1.08382712,0.,0.7662802131
C 0.8676768759,1.2865863539,0.
C 0.8676768759,-1.2865863539,0.
H 0.1644433784,2.1198103843,0.
H 0.1644433784,-2.1198103843,0.
H 1.5056677295,1.3459546611,0.8865049416
H 1.5056677295,1.3459546611,-0.8865049416
H 1.5056677295,-1.3459546611,-0.8865049416
H 1.5056677295,-1.3459546611,0.8865049416

DFDO G2MP2= -387.70088\G2=-387.71245
Charge = 0 Multiplicity = 1
O -0.1235870926,0.,-1.2765917373
C -0.04859426,0.,0.0758273281
O 1.2114950574,0.,-0.4209987638
F -0.4673165643,-1.079184813,0.7292088911
F -0.4673165643,1.079184813,0.7292088911

TFDO G2MP2= -565.31741
Charge = 0 Multiplicity = 1
C 0 0.17497 -0.6684 0.27099
O 0 0.16035 -0.66329 1.66593
O 0 1.45232 -0.66329 0.83175
C 0 -0.22319 0.66084 -0.34568
C 0 -0.28679 -1.89503 -0.44417
F 0 0.22767 1.70296 0.35261
H 0 0.06946 -2.76514 0.10758
F 0 0.26528 0.73799 -1.60329
F 0 -1.5704 0.73799 -0.41806
H 0 -1.37783 -1.90856 -0.49696
H 0 0.11412 -1.90856 -1.46026

1,2-dioxacyclobutane (dioxetane) G2MP2= -228.57919\G2=-228.58482
Charge = 0 Multiplicity = 1

O	-0.7644505658,0.2550670623,-0.7154291539
O	-0.7645179126,-0.2547244694,0.7154787055
C	0.6713992533,-0.0141240835,0.7534679793
C	0.671355959,0.0138233148,-0.7535114611
H	1.1954973577,-0.8227680721,1.26753682
H	0.8922214408,0.9529139763,1.2155225772
H	0.8917146235,-0.9533138861,-1.2155798598
H	1.1957831313,0.8222318513,-1.26761506

methyldioxetane G2MP2=-267.81324\G2=-267.81979
Charge = 0 Multiplicity = 1

O	-0.8949723412,-0.7047429975,-1.0772197547
C	-1.1274599073,-0.154736379,0.2489338193
C	0.3647262076,-0.1507711664,0.4842863031
O	0.5487704721,-0.2422289909,-0.964200167
H	-1.7569048768,-0.8158619032,0.8496443483
H	-1.5612149984,0.8500233729,0.1871808399
H	0.710077859,-1.0807130577,0.9529829297
C	1.0475069458,1.0607666518,1.0566501614
H	0.8652337311,1.129300004,2.1334448678
H	2.1271381066,0.9958449157,0.8979166106
H	0.6766456553,1.9656279365,0.5709680745

1,1-dimethyldioxetane G2MP2 -307.048051
Charge = 0 Multiplicity = 1

O	-1.1602015813,-0.0419917044,-1.2570064824
O	-1.2016230415,-0.0210837503,0.261867716
C	0.2722344684,0.0043814738,0.2662120414
C	0.2261124077,-0.4694398199,-1.1726932704
H	0.3092509422,-1.5564101677,-1.2852801389
H	0.8473984994,0.0479256239,-1.9096601559
C	0.7523106332,1.4309441291,0.4242648893
H	1.8405229906,1.4887209163,0.3186758023
H	0.2836444589,2.0599840178,-0.3356113852
H	0.4762347808,1.8096581613,1.4118619459
C	0.8038888506,-0.9381846736,1.3166070387
H	0.3964631655,-1.9405280159,1.1699275248
H	1.8965230356,-0.9840142425,1.2726898062
H	0.5172809498,-0.5869393122,2.3121625383

F_2COO G2MP2=-387.63136\G2=-387.64354
Charge = 0 Multiplicity = 1

O	-0.8630899131,0.,-1.6550121998
O	-0.9414261282,0.,-0.2219494675
C	0.1483141911,0.,0.3519025593
F	1.3020201657,0.,-0.2185421833

F 0.2031179659,0.,1.652350848

1,2-dioxacyclopentane G2MP2=-267.83679\G2=-267.84329
Charge = 0 Multiplicity = 1
O -0.9584491683,0.4543507307,-0.6303281494
O -1.0158283768,-0.3169572213,0.6245065466
C 0.2657209466,-0.0121358221,1.184381571
C 1.2431671641,-0.0864846528,0.0036614897
C 0.2717772201,-0.0252963805,-1.1827935362
H 0.2483638305,0.9866439025,1.6330544806
H 0.4348767797,-0.7669207418,1.9559404896
H 1.9413394803,0.7533278586,0.0127945557
H 1.8184153224,-1.0148561807,-0.0017238493
H 0.5483549976,0.6984181588,-1.9530916235
H 0.1188779656,-1.0122599406,-1.6318983778

1,3-dioxacyclopentane G2MP2=-267.9132954\G2=-267.9197736
Charge = 0 Multiplicity = 1
O -0.98259849,0.0795091224,-0.6990747995
C -0.8143717939,0.6680628138,0.5831500273
O 0.4819290113,0.3315433396,1.0574916263
C 0.9566279539,-0.7110514276,0.2041027565
C 0.3187447796,-0.3354435422,-1.1172836545
H -1.5993325586,0.2681132,1.2362399701
H -0.8756868849,1.7619772716,0.5360805619
H 2.0475030546,-0.6804558987,0.2132463335
H 0.6070255862,-1.6942397408,0.5457599871
H 0.8629227695,0.4880702958,-1.5982225566
H 0.1969182258,-1.1612918884,-1.8202536857

1,2-dioxacyclohexane G2MP2=-307.0667782\
Charge = 0 Multiplicity = 1
C -1.1691235864,-0.4195083686,-0.7140449097
C -1.1676656929,-0.2221153587,0.7999494883
C 0.2513233844,-0.3580063,1.3283296815
C -0.057791343,0.411145331,-1.33544433
H 0.3332405863,-0.0640420592,2.3798242141
H -1.5303752348,0.7826743759,1.0441493462
H -1.8298205053,-0.9425287742,1.2937700949
H 0.090574315,0.1804107083,-2.3954043676
H -2.1380286833,-0.146943321,-1.1479048836
H -0.2376664483,1.4867230203,-1.2216223377
H -0.9843518194,-1.4731554017,-0.9517033273
H 0.6378721632,-1.3768365712,1.2069097938
O 1.1164854241,0.5595818048,0.6509683227
O 1.1982769576,0.0759939703,-0.7360630868

1,2-4,5-tetraoxacyclohexane G2MP2(0 K)= -378.796818
Charge = 0 Multiplicity = 1

C	-1.2831376183,0.0000124496,-0.2210378426
C	1.2831375751,-0.0000125356,0.2210376476
H	-2.1145771226,0.0000238858,-0.9295043381
H	1.601368346,-0.0000089836,-0.8243026495
H	2.1145775191,-0.0000239795,0.929503642
H	-1.6013690669,0.0000087074,0.8243022655
O	-0.5353904558,1.1651061129,-0.5078262476
O	-0.535410544,-1.1650906675,-0.5078404843
O	0.5353903295,-1.1651060003,0.507826486
O	0.5354107433,1.1650906655,0.5078405271

1,1-dimethyl-2,3-dioxacyclohexane G2MP2=-385.53089
Charge = 0 Multiplicity = 1

C	-1.06981	-0.76255	-0.22906
C	-0.99917	-0.83146	1.29477
C	0.45549	-0.87082	1.72879
C	-0.11604	0.29197	-0.79552
H	0.57046	-0.76293	2.81263
H	-1.47873	0.04304	1.74631
H	-1.5291	-1.71772	1.66374
H	-2.09314	-0.5612	-0.56812
H	-0.77388	-1.73404	-0.64404
H	0.95316	-1.79213	1.40202
O	1.1558	0.25732	1.19844
O	1.20471	0.04006	-0.25732
C	-0.54733	1.7184	-0.49541
H	-1.50655	1.93195	-0.97735
H	-0.64443	1.88902	0.57665
H	0.20347	2.41182	-0.88299
C	0.10235	0.08794	-2.28553
H	0.50135	-0.91135	-2.47774
H	-0.84776	0.19562	-2.8171
H	0.80798	0.82807	-2.67122

1,1-difluoro-2,3-dioxacyclohexane G2MP2(0 K)= -505.40115/ G2=-505.41476
Charge = 0 Multiplicity = 1

C	1.290165	-0.312261	0.063792
C	1.130613	0.185397	-1.371045
C	-0.220486	-0.261078	-1.898293
C	0.038543	-0.016079	0.848548
H	-0.465951	0.196898	-2.861185
H	1.170967	1.278282	-1.390572
H	1.940996	-0.194534	-2.001747

H	2.141200	0.148587	0.572340
H	1.420762	-1.398202	0.086031
H	-0.296645	-1.351344	-1.983085
O	-1.255405	0.225211	-1.034748
O	-1.119661	-0.510522	0.231134
F	-0.083410	1.317985	1.080303
F	0.045208	-0.648326	2.047377

RADICALS

CH_3OCH_2 • G2MP2=-154.0894701\G2=-154.0933741

Charge = 0 Multiplicity = 2

O	-0.4688748064,-0.2985421822,-0.0761684862
C	0.8838322707,-0.7293023776,0.0296489657
H	1.4728086279,-0.377004025,-0.8225832805
H	1.3363196089,-0.3638409801,0.9588904452
H	0.8621097505,-1.818151294,0.0381080125
C	-0.6119835168,1.0565613726,-0.0389039078
H	-1.6483978183,1.3635504234,-0.0733238032
H	0.0970657585,1.6202293632,0.5637861681

cyclopropane radical G2MP2=-116.9553032\G2=-116.9577311

Charge = 0 Multiplicity = 2

C	0.8441089558,-0.0060563702,0.0554144993
C	-0.432733997,0.1175233784,0.7703974511
C	-0.4866472562,-0.0071586578,-0.6919177504
H	1.4662039896,0.8777347002,-0.0595381107
H	1.4070126586,-0.9329616452,0.1336999204
H	-0.8628670792,-0.5117233066,1.5371926656
H	-0.8452990879,-0.9348296305,-1.1311652018
H	-0.7134166968,0.8759297794,-1.2835544736

cycbutane radical G2MP2=-156.1955646\G2=-156.1989294

C	0.8173641927,-0.09347373,-0.7276754435
C	0.6941700747,0.0887931679,0.8106370431
C	-0.8447785857,-0.0934733111,0.6956619558
C	-0.6786070118,0.0142382923,-0.7924624683
H	1.403500709,0.658407906,-1.2691376457
H	1.2045832519,-1.0818091586,-1.0134005361
H	0.9715140778,1.0943187958,1.1345131043
H	1.2249018791,-0.6379767342,1.4304144344
H	-1.4699818211,0.6584086301,1.1915024417
H	-1.1866831316,-1.0818085559,1.0343049434
H	-1.377777635,-0.1339613024,-1.6089388292

cyclopentane radical G2MP2=-195.4567433\G2=-195.460916
Charge = 0 Multiplicity = 2

C	-0.9800822154,0.2693181772,-0.7143596132
C	-1.0464062191,-0.0750660297,0.7823508439
C	0.3857987634,0.0004524145,1.209969006
C	1.3061402363,0.0752494816,0.0321877191
C	0.3856947278,-0.2698073528,-1.149710663
H	-1.8112195102,-0.1479336231,-1.2906742828
H	-1.0014965535,1.3577517637,-0.8411202754
H	-1.4534225984,-1.089478979,0.9226331364
H	-1.7025844316,0.5987650154,1.3467808434
H	1.7192749168,1.0895741272,-0.0896058254
H	2.1679090279,-0.5985626163,0.1130100273
H	0.7297536697,0.1470519315,-2.1009615714
H	0.329928796,-1.3583015159,-1.2649710276
H	0.7149849251,0.000253751,2.2422852189

$CH_3CH_2CH_2CH_2$• G2MP2=-157.4160359\G2=-157.4196158
Charge = 0 Multiplicity = 2

C	-0.4430400382,0.0000814874,-0.5733752675
H	-1.0991803808,-0.8774981148,-0.5664988482
H	-1.0989345602,0.8778442171,-0.5664420727
C	0.4067732101,-0.0000788071,0.7085166574
H	1.0622886217,0.8792170279,0.6905399488
H	1.0620425584,-0.8795576974,0.6904783607
C	-0.4094116717,-0.0000088619,1.9558254385
H	-0.816697605,0.9240296822,2.3473102027
H	-0.8169964676,-0.9239576708,2.3472112737
C	0.4124553101,0.0000024408,-1.8353222775
H	1.0566197915,0.8836910691,-1.8696762638
H	1.0563725738,-0.8838641588,-1.8697331428
H	-0.2061753939,0.0001180901,-2.7370567639

$CH_3CH_2OCH_2CH_2$• G2MP2=-232.5380551\G2=-232.543686
Charge = 0 Multiplicity = 2

O	-0.1224073177,-0.1051483711,-0.2501145268
C	-0.1740156994,1.311036126,-0.176159864
C	-0.9420450152,1.8159028681,-1.3396487235
H	0.8444712711,1.7352194724,-0.1655850407
H	-0.6457246807,1.6168532488,0.7782239393
H	-1.6966963534,1.1835038975,-1.7856126997
H	-0.9165041757,2.8664066907,-1.5967384528
C	0.5658257061,-0.6676420576,0.8566950862
C	0.5596334812,-2.169991629,0.685268591
H	0.0710043239,-0.3778224129,1.7970830324

H 1.596598121,-0.2820509254,0.8968735708
H 1.0803489643,-2.6543618839,1.5158209555
H -0.4671241901,-2.5393809772,0.6515537823
H 1.0564944254,-2.4430119859,-0.2476334114

$CH_3OOCH_2CH_2$• G2MP2=-268.35852/G2=-268.36557
Charge = 0 Multiplicity = 2

O	-0.331082	0.530501	-1.136200
O	-0.285484	0.322077	0.320640
C	1.024458	-0.198647	0.567411
C	-1.436158	-0.252704	-1.565997
H	1.761505	0.477397	0.108067
H	1.136690	-1.185098	0.099771
H	-2.361448	0.080440	-1.088570
H	-1.273365	-1.315482	-1.362107
C	1.172927	-0.267275	2.041677
H	0.806769	0.546501	2.651953
H	1.782707	-1.032842	2.500154
H	-1.487685	-0.079785	-2.643336

ethyl radical G2MP2=-78.9681136\G2=-78.9701607
Charge = 0 Multiplicity = 2
C 0.0052128762,-0.0000055933,-0.6948968436
C -0.0364225684,0.0000054711,0.7938602398
H 1.0362218363,0.0000318608,-1.0757822915
H -0.4865991665,-0.884554064,-1.1071454486
H -0.4866676244,0.8844981287,-1.1071604613
H 0.0621715113,-0.9236873745,1.3481618895
H 0.0621315963,0.9237121883,1.3481459349

$CH_3CH_3CH_2$• G2MP2=-118.1912529\G2=-118.1940267
Charge = 0 Multiplicity = 2
C 0.6157737086,1.0738531231,-0.0365923558
H 0.0832629504,1.6125581475,0.7509701953
H 1.5745282435,0.7444609004,0.3712254024
H 0.8145224996,1.7727929605,-0.8538782141
C -0.2079599765,-0.126272659,-0.5279225932
H 0.3372440271,-0.6227796172,-1.3377383649
H -1.1452172668,0.2401904589,-0.9601633202
C -0.5033871789,-1.1078529406,0.5556060796
H 0.2341892103,-1.8469468489,0.842688914
H -1.3250889829,-0.9386411422,1.2403486035

ethyl propyl ether radical (Cs) G2MP2=-271.76416 a.u.
Charge = 0 Multiplicity = 2
C 0 0.75619 0. 0.19072

C	0	0.78062	0.	1.71659
C	0	2.1667	0.	2.26569
O	0	-0.60185	0.	-0.21825
H	0	1.27709	0.88788	-0.20082
H	0	1.27709	-0.88788	-0.20082
H	0	0.22774	0.88091	2.05807
H	0	0.22774	-0.88091	2.05807
H	0	2.71717	0.92467	2.38331
H	0	2.71717	-0.92467	2.38331
C	0	-0.73175	0.	-1.63255
H	0	-0.23632	-0.88692	-2.05738
H	0	-0.23632	0.88692	-2.05738
C	0	-2.20851	0.	-1.95858
H	0	-2.68598	0.88585	-1.53535
H	0	-2.68598	-0.88585	-1.53535
H	0	-2.36413	0.	-3.04092

neopentane radical G2MP2=-196.6475178\G2=-196.6518337
Charge = 0 Multiplicity = 2

C	-0.8720316516,0.0000015565,1.2330052429
C	0.0512688672,-0.0000000976,0.0032067772
H	-0.6972828627,-0.88599008,1.8509554046
H	-0.6972794976,0.8859924202,1.8509555599
H	-1.9231890021,0.000003579,0.9229342758
C	-0.2284204625,1.2505317905,-0.8332734532
H	0.4100152569,1.2747853882,-1.721432529
H	-1.2731388029,1.2713184293,-1.1604985007
H	-0.0374543947,2.1586967813,-0.2521948781
C	1.4790794403,-0.0000028548,0.4519746744
H	1.955051454,0.9259845041,0.7567849018
H	1.9550478506,-0.9259920691,0.7567848909
C	-0.2284252198,-1.2505307797,-0.8332736529
H	0.4100104149,-1.274786674,-1.7214327263
H	-0.0374626199,-2.1586965901,-0.2521952194
H	-1.2731436386,-1.2713133788,-1.1604987096

$CH_3CH_2OCH_2$• G2MP2=-193.3187895\G2=-193.3235328
Charge = 0 Multiplicity = 2

O	0.0578159892,0.7370398591,-0.1052847575
C	-0.0992137221,-0.6831192071,-0.0434969516
C	0.8402089084,-1.1985653869,1.0216052502
H	0.1305895559,-1.1180446801,-1.0235125659
H	-1.1438897919,-0.9226282003,0.1980033747
H	0.7587667484,-2.2854103448,1.1067238324
H	1.8711712709,-0.9434698086,0.7696639382

H 0.5979637013,-0.7517894558,1.9877052788
C -0.7806135994,1.3481449192,-0.9900348256
H -0.6790427685,2.4250087366,-0.9804619126
H -1.7603761508,0.9012529287,-1.1442847233

CH3(CH2•)CH3 G2MP2=-118.195964\G2=-118.1988786
Charge = 0 Multiplicity = 2
C 0.533498482,-0.107505112,0.
H 1.4633275646,-0.6670468207,0.
C -0.1915613442,0.0584834242,-1.2914834145
H -0.8816596415,-0.7775631715,-1.4835715307
H -0.7978413881,0.9707860088,-1.2865052828
H 0.4967098665,0.1119153637,-2.1387006943
C -0.1915613442,0.0584834242,1.2914834145
H -0.7978413881,0.9707860088,1.2865052828
H -0.8816596415,-0.7775631715,1.4835715307
H 0.4967098665,0.1119153637,2.1387006943

CH_3CH_2OO• (State=2-A") G2MP2=-229.1704323\G2=-229.1772647
C
C,1,B1
O,2,B5,1,A4
H,1,B2,2,A1,3,D3,0
H,1,B4,2,A3,4,D1,0
H,1,B4,2,A3,4,-D1,0
H,2,B6,1,A5,3,D4,0
H,2,B6,1,A5,3,-D4,0
O,3,B7,2,A6,1,D5,0
Variables:
B1=1.50935986
B2=1.09275874
B4=1.09155707
B5=1.46045185
B6=1.09169809
B7=1.3109156
A1=109.73657064
A3=110.65216261
A4=106.4978771
A5=112.94843524
A6=110.6732988
D1=119.70900006
D4=117.57396934
Constants:
D5=180.
D3=180.

(CH3)3C• G2MP2=-157.426099\G2=-157.4298558
Charge = 0 Multiplicity = 2

C	0.2219505088,-0.3854164833,-1.4100265339
C	0.0903764827,-0.15682406,0.0598994904
H	1.271858304,-0.4308423212,-1.7155838717
H	-0.2652533715,-1.316598011,-1.7154254155
H	-0.246525551,0.4274581361,-1.9888806344
C	-1.2350349928,-0.4209120395,0.695344764
C	0.9835608112,0.8575589271,0.695114147
H	-1.1501631111,-0.4898383552,1.7842805089
H	-1.9546138892,0.3858401699,0.4793259708
H	-1.6778250609,-1.3510168655,0.3257813112
H	0.6463341776,1.8846460351,0.4790648306
H	1.0008172004,0.7496570758,1.7840561005
H	2.0102544428,0.7742560703,0.3253899942

Dioxirane radical   G2MP2=--188.704190\G2=-188.7092418
Charge = 0 Multiplicity = 2

O	-0.369694793,0.0560259481,0.7802713842
C	0.7175428093,-0.2187532742,-0.0000118461
O	-0.3697225069,0.0560182076,-0.7802585924
H	1.6100815429,0.4161663996,-0.0000312573

DMDO CH3-radical (methyl dioxirane radical) G2MP2=-227.9428867\G2=-227.9489675
Charge = 0 Multiplicity = 2

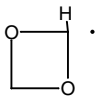
C	0.,0.4321672844,0.0780797698
O	0.7808251056,-0.0900746227,-0.9227103517
O	-0.7808251056,-0.0900746227,-0.9227103517
C	0.,-0.0853142876,1.4737247833
H	0.,-1.180066505,1.451086273
H	0.8873959158,0.2700712437,2.0007260178
H	-0.8873959158,0.2700712437,2.0007260178

DFDO F-radical \G2MP2=-287.8649447\G2=-287.873191\
Charge = 0 Multiplicity = 2

O	-0.2469937334,0.324510687,-1.0711956732
C	-0.180842746,0.287042833,0.2821900527
O	1.0764313702,0.3245107709,-0.2230729152
F	-0.6167160687,-0.7682698513,0.9623342657

Dioxetane radical G2MP2=-227.91596/G2=-227.92158/
MP2/6-311+G(3DF,2P)= -227.8619449
Charge = 0 Multiplicity = 2

O	-0.7351065289,-0.0629181023,-0.7316458453
O	-0.7334093848,-0.0206994543,0.7816062325
C	0.6598143683,-0.0539339633,0.7740252178
C	0.7273257841,0.0432000703,-0.7033994117
H	1.1757150081,0.5138464058,1.5423617426
H	1.1897641845,-0.7842912707,-1.2498087627
H	1.0598072035,1.0037886761,-1.1159909143



\G2MP2=-228.0114279\G2=-228.0170962\
Charge = 0 Multiplicity = 2

C	0.6380883484,0.0748870139,-0.678634326
O	-0.7943848221,-0.0073408215,-0.6691544997
C	-0.6798901973,0.0225516494,0.723092368
O	0.7167634943,-0.0073405859,0.7517081121
H	1.1007117156,-0.7853258888,-1.1706539678
H	1.0082491445,1.0255681899,-1.0723163584
H	-1.237179145,-0.7074230214,1.3157931753

1,2-dioxacyclopentane α-radical MP2/6-311+G(3DF,2P)=-267.1171164
G2MP2=-267.18442
Charge = 0 Multiplicity = 2

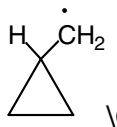
O	-0.9872941482,0.1398517104,-0.7212113093
O	-0.9896188486,0.1204758805,0.7875633316
C	0.3258142906,0.1572964895,1.1750891
C	1.2257186575,0.1592968576,-0.0199394903
C	0.2757475649,-0.4394698644,-1.0495912501
H	0.5080488091,-0.4312510039,2.0708163851
H	1.5064505945,1.177808341,-0.3107980426
H	2.1352503249,-0.4273434466,0.1325615685
H	0.4684080239,-0.1310406282,-2.0801580088
H	0.2334631434,-1.5335348859,-0.9765882381

1,2-dioxacyclopentane β-radical \G2MP2=-267.1762144\
Charge = 0 Multiplicity = 2

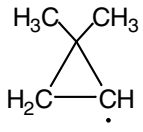
O	-1.0066720454,0.0159499961,-0.6611285622
O	-0.871738526,-0.3018516649,0.7768409929
C	0.3415445336,0.3826216747,1.1208850236
C	1.2124047173,0.160643869,-0.0663100923
C	0.3056760549,-0.2907367722,-1.1601376117
H	0.1434490424,1.4490332044,1.3095441994
H	0.6959653876,-0.0896678366,2.0433325134
H	0.4073705005,0.271441297,-2.0942198225
H	0.393350136,-1.3670866047,-1.3693291637

H 2.2293976696,0.5083206614,-0.1816510889

\G2MP2=-156.1874294\G2=-156.1907726
Charge = 0 Multiplicity = 2
C -0.7649271322,-0.0730437371,-0.9696315978
C 0.000001469,0.4049295181,0.1895671929
C 0.7649253991,-0.073048826,-0.9696325771
H -1.283960511,-1.027781293,-0.8978726706
H -1.2576897082,0.6476522641,-1.6175699527
H 1.2576919393,0.6476438967,-1.6175715638
H 1.2839525167,-1.0277898364,-0.8978743225
C 0.0000008836,-0.0444420382,1.6019608979
H 0.8882387817,0.3089496539,2.1326735385
H -0.8882338485,0.308955793,2.1326747547
H -0.0000028845,-1.1439999791,1.6519567218

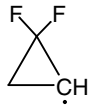


\G2MP2=-156.2002795\G2=-156.2035497\
Charge = 0 Multiplicity = 2
C -0.7464796728,-0.1359284322,-0.9015454729
C -0.0000260502,0.4900543244,0.2630324489
C 0.7465209939,-0.1359051541,-0.901518142
H -1.2587547984,-1.0723411397,-0.7079317211
H -1.2659579938,0.5282554996,-1.5840916213
H 1.2660070066,0.5283080257,-1.5840303964
H 1.2588234371,-1.0722966273,-0.7078782459
C -0.0000505661,-0.1613563446,1.5691436259
H -0.0000605145,-1.2420165243,1.6437154959
H 0.0001846303,0.4126955349,2.4849616226
H -0.0000299961,1.5762088699,0.2805801065



\G2MP2=-195.4128985\G2=-195.417001\
Charge = 0 Multiplicity = 2
C -0.0223215589,-0.0223085162,-1.4041090264
C -0.0197797006,-0.0147044798,0.1239771222
C 1.2373356181,0.0091458345,-0.6400255403
H -0.318862327,-0.9513640191,-1.8872094993
H -0.3390686482,0.8717335748,-1.9389623414
H 2.0303890572,0.7471030226,-0.6517030911
C -0.4228055743,-1.2987055333,0.8160401817

H	0.0135582769,-1.3471249795,1.8192716591
H	-1.5120251394,-1.3589572615,0.9140293617
H	-0.0766520687,-2.1711075759,0.2557317553
C	-0.4545341783,1.244480154,0.8393331962
H	-1.5432509313,1.2632261879,0.9619632571
H	-0.000887027,1.3011079457,1.8346009655
H	-0.1605688289,2.1379383498,0.2809823331



\G2MP2=-315.2630005\G2=-315.2713656\
Charge = 0 Multiplicity = 2

C	-0.0572381133,-1.3405580405,-0.0745844038
C	0.0207410094,0.1036589078,-0.1154962011
C	0.0132599582,-0.5785649194,1.212180499
H	-0.7918567303,-2.0422644925,-0.4425644782
H	0.9573785084,-0.5782864604,1.7541233532
H	-0.8767017818,-0.5204540537,1.835253798
F	-1.0575407694,0.8320399319,-0.5028014997
F	1.1520522002,0.7272699925,-0.5282442822

$CH_3CF_2CH_2\bullet$ MP2/6-311+G(3df,2p)=-316.4486002\G2MP2=-316.5172249
Charge = 0 Multiplicity = 2

C	-0.0000052942,1.0010826647,1.1463572973
C	-0.0000001961,0.009910567,0.0424651462
H	0.9360870469,1.4297444401,1.4730805668
H	-0.9361006531,1.4297444401,1.4730719205
C	0.0000062685,0.5747342208,-1.3573095948
H	0.0000095468,-0.2547837884,-2.0671582753
H	-0.8906958437,1.1855581558,-1.5119160516
H	0.8907098087,1.1855581558,-1.5119078245
F	-1.108752566,-0.8050103399,0.1753144668
F	1.1087509467,-0.8050103399,0.1753247079

$FCH_2CH_2(CH\bullet)$ F MP2/6-311+G(3df,2p)=-316.4284505\G2MP2=-316.494 8645
Charge = 0 Multiplicity = 2

C	0.1136136074,0.2817994216,1.4758634555
C	-0.6632006906,0.2800251067,0.2125362355
H	0.6310189256,1.159391582,1.8508654488
C	0.2290622206,0.1676676813,-1.0160879462
H	-1.3603086143,-0.5641398484,0.2076213685
H	-1.2519827515,1.1993259409,0.1470589015
H	0.9108054093,1.0200390007,-1.0918572948
H	0.810828147,-0.7565689135,-0.9869229746
F	0.8165143609,-0.8635002133,1.6955970316
F	-0.5739823543,0.1485001,-2.1578899115

FCH_2 ($CH\bullet$) CH_2F MP2/6-311+G(3df,2p)=-316.4226017\G2MP2=-316.490275
Charge = 0 Multiplicity = 2

C	-0.4519513108,0.062583573,-1.3059025475
C	-0.2649364448,-0.0154845825,0.1627461858
H	0.5099913272,0.0318245342,-1.8317358569
H	-0.9751014647,0.9792266573,-1.6153263969
C	0.8286576889,0.7203670964,0.8414010951
H	-1.091936953,-0.3728446524,0.7654228796
H	1.7589793037,0.6733657873,0.2625461948
H	0.5857985471,1.7809813797,1.0019642444
F	-1.2259639436,-1.0157302498,-1.7405093458
F	1.0639250146,0.1604691135,2.0991382941

$FCH_2CH_2\bullet$ G2M P2=-178.1158595\G2=-178.1207909
Charge = 0 Multiplicity = 2

C	0.0000052581,-0.4423286828,-0.3160400022
C	0.0000056298,-0.4634300631,1.1664875345
H	0.8897152337,-0.9284778134,-0.7238667349
H	-0.88969333,-0.928498857,-0.7238665385
H	0.925923146,-0.3472095928,1.7135237759
H	-0.925914911,-0.3472338785,1.7135237573
F	-0.0000106081,0.8873302908,-0.7868888282

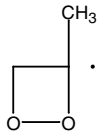
$CH_3CF_2\bullet$ G2MP2=-277.2865785\G2=-277. 2945798
Charge = 0 Multiplicity = 2

C	1.207261063,-0.2947405435,-0.6073047167
H	1.7591988746,0.5870067825,-0.2624809186
H	1.7094733538,-1.1911078928,-0.2436688024
H	1.1956128227,-0.3010438875,-1.6971429328
C	-0.1856334135,-0.2515686556,-0.0884243375
F	-0.2817490147,-0.3182849006,1.2535650493
F	-0.9175899795,0.7830626996,-0.5449353848

HOOCF2 G2MP2(0 K)= -388.236386/G2(0 K)= -388.248008
Charge = 0 Multiplicity = 2

O	-0.1440568281,-0.3893889055,1.7716128716
O	-0.8099175842,-0.0708505783,0.5104360353
H	0.0212312465,0.5190957669,2.0969579086
C	0.1483744366,-0.2377563884,-0.4525667319
F	-0.4457634064,-0.0877971075,-1.6319320897
F	1.1924653433,0.5977258224,-0.3278399961

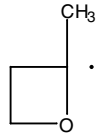
3-methyldioxetane radical \G2MP2=-267.1615663\



Charge = 0 Multiplicity = 2

O	-0.1825185867,0.1318363125,1.5407986158
O	-1.0714870354,-0.0281434019,0.3247765703
C	0.0572187415,-0.3401927443,-0.4505020777
C	0.9820059559,-0.0328936468,0.6712688801
H	1.5438979326,0.9079650555,0.58334818
H	1.6367862111,-0.8309961028,1.0344001929
C	0.0683359321,0.1103860381,-1.8622956643
H	0.1083932332,1.2061028861,-1.9352414389
H	0.9333935338,-0.3049102507,-2.3851342834
H	-0.8357897112,-0.2315027543,-2.3728009684

2-methyloxetane radical \G2MP2=-231.3392157



Charge = 0 Multiplicity = 2

C	-0.5120031108,-0.1403101045,-1.4202473228
O	-0.0809969783,-1.0471148499,-0.3583010272
C	-0.1016485986,0.019178243,0.553837598
C	-0.3285168853,1.0725462924,-0.4973555306
H	0.1550010637,-0.2127696709,-2.2825816844
H	-1.5416224525,-0.3502112938,-1.7219776172
H	0.5540801158,1.6790298208,-0.7371117483
H	-1.1897426354,1.7330542802,-0.3677171175
C	0.8429699395,-0.0160969422,1.695607705
H	0.6258485332,0.7959896049,2.3943818779
H	0.7533932129,-0.9666696214,2.2285409157
H	1.8862099194,0.086590747,1.3618188943