Electronic Supporting Information

The kinetics of carbonyl radical ring closures.

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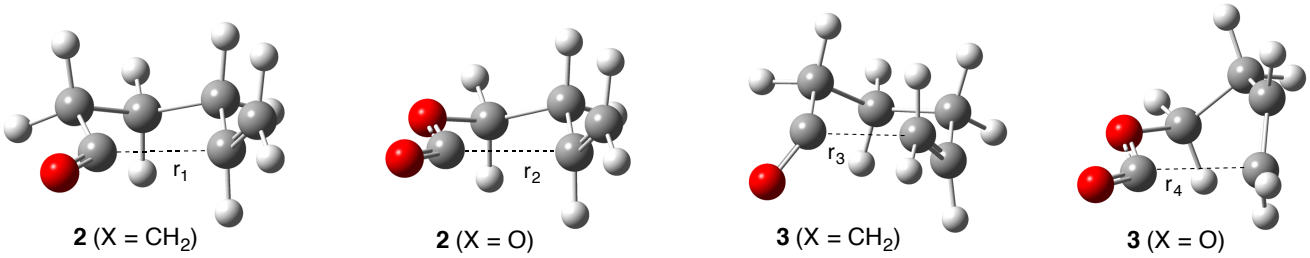
Table S1, Figures S1 – S3, Gaussian Archive Entries of all transition states calculated in this work (49 pages).

Level of Theory	$\Delta E_1^{\ddagger}$	$\Delta E_2^{\ddagger}$	$\Delta E_3^{\ddagger}$	$\Delta E_4^{\ddagger}$	$\Delta E_1^{\ddagger}$	$\Delta E_2^{\ddagger}$	$\Delta E_3^{\ddagger}$	$\Delta E_4^{\ddagger}$
X = CH_2					**X = O**			
HF/6-31G(d)	51.7 (50.0)[a]	112.2 (105.8)[a]	67.5 (63.6)[a]	146.5 (139.5)[a]	35.3 (30.2)[a]	131.5 (124.8)[a]	60.3 (57.0)[a]	163.3 (156.5)[a]
HF/6-311G(d,p)	57.9 (51.8)[a]	108.9 (102.5)[a]	74.7 (70.8)[a]	142.2 (135.5)[a]	40.3 (35.5)[a]	144.4 (138.0)[a]	66.6 (63.3)[a]	159.4 (152.6)[a]
B3LYP/6-31G(d)	32.4 (30.2)[a]	75.1 (71.5)[a]	39.2 (39.7)[a]	96.0 (90.9)[a]	21.3 (19.7)[a]	92.7 (89.4)[a]	41.3 (41.0)[a]	105.5 (100.7)[a]
BHandHLYP/6-311G(d,p)	47.7 (44.5)[a]	94.4 (90.6)[a]	57.3 (57.0)	124.8 (121.1)[a]	33.8 (31.6)[a]	113.6 (110.4)[a]	55.5 (54.7)[a]	146.5 (142.1)[a]
BHandHLYP/6-311++G(d,p)	47.1 (44.2)[a]	94.5 (90.5)[a]	56.8 (56.8)[a]	125.4 (121.7)[a]	33.7 (31.6)[a]	113.2 (109.9)[a]	55.3 (54.7)[a]	146.5 (142.0)[a]
BHandHLYP/cc-pVDZ	45.6 (42.4)[a]	96.5 (93.0)[a]	55.4 (54.9)[a]	129.2 (125.5)[a]	32.1 (29.7)[a]	116.4 (113.1)[a]	53.8 (52.8)[a]	151.1 (146.8)[a]
BHandHLYP/aug-cc-pVDZ	45.5 (42.5)[a]	97.6 (93.6)[a]	53.7 (53.8)[a]	127.7 (124.3)[a]	31.2 (29.0)[a]	118.3 (114.6)[a]	51.6 (51.1)[a]	150.4 (146.2)[a]
BHandHLYP/cc-pVTZ	48.7 (45.7)[a]	92.8 (89.0)[a]	58.0 (57.9)[a]	123.3 (119.8)[a]	34.7 (32.4)[a]	113.0 (109.5)[a]	55.9 (55.2)[a]	145.9 (141.7)[a]
BHandHLYPaug-cc-pVTZ	48.0 (45.1)[a]	92.3 (88.5)[a]	57.4 (57.4)[a]	123.1 (119.6)[a]	34.2 (32.0)[a]	112.4 (108.9)[a]	55.4(54.8)[a]	145.2 (141.1)[a]
MP2/6-311G(d,p)	73.0 (67.9)[a]	122.9 (121.8)[a]	78.8 (78.6)[a]	137.4 (136.5)[a]	59.4 (51.3)[a]	139.4 (137.6)[a]	81.4 (74.9)[a]	162.1 (159.6)[a]
MP2/6-311++G(d,p)	72.4 (69.8)[a]	121.5 (120.6)[a]	78.8 (76.9)[a]	137.9 (136.9)[a]	58.8 (51.9)[a]	138.5 (136.6)[a]	80.6 (75.3)[a]	161.4 (158.8)[a]
MP2/cc-pVDZ	72.8 (61.4)[a]	123.0 (122.1)[a]	80.4 (71.6)[a]	140.5 (139.1)[a]	59.0 (47.6)[a]	138.3 (136.5)[a]	81.6 (71.8)[a]	163.8 (161.5)[a]
MP2/aug-cc-pVDZ	69.0 (61.4)[a]	119.1 (118.8)[a]	72.4 (67.7)[a]	134.3 (133.9)[a]	54.2 (45.0)[a]	138.7 (137.4)[a]	73.6 (66.0)[a]	160.6 (158.5)[a]
ROMP2/6-311++G(d,p)[b]	44.9	93.1	54.6	112.3	33.9	112.4	52.7	132.9
ROMP2/6-311++G(d,p)[c]	47.1	93.9	49.0	107.9	35.3	112.6	54.4	133.5
ROMP2/aug-cc-pVDZ[d]	40.6	90.4	42.6	104.5	29.2	112.2	45.8	132.0
ROMP2/aug-cc-pVDZ[e]	42.8	91.0	45.2	105.5	33.3	115.1	47.3	132.2
QCISD/6-311++G(d,p)[b]	49.3	95.6	58.5	118.3	35.8	112.5	57.1	137.9
QCISD/6-311++G(d,p)[c]	51.7	96.7	63.7	122.5	37.9	113.5	60.0	139.9
QCISD/aug-cc-pVDZ[d]	44.9	93.3	52.4	115.4	31.0	112.9	50.4	137.6
QCISD/aug-cc-pVDZ[e]	47.6	94.7	56.6	118.6	35.6	116.6	53.1	139.5
CCSD(T)/6-311++G(d,p)[b]	45.2	90.0	52.3	109.2	32.1	106.2	52.3	129.8
CCSD(T)/6-311++G(d,p)[c]	48.5	91.4	59.8	115.2	34.7	107.4	55.6	132.0
CCSD(T)/aug-cc-pVDZ[d]	40.4	87.3	45.8	106.1	27.0	106.3	45.2	129.3
CCSD(T)/aug-cc-pVDZ[e]	43.8	89.0	50.4	109.2	33.2	111.5	48.1	131.2
G3(MP2)-RAD[f]	34.1		41.7		23.1		41.9	
G3(MP2)-RAD[g]	36.7		44.1		25.5		44.3	

[a]Values in parentheses are zero-point energy (ZPE) corrected. [b]Single point calculation optimised at BHandHLYP/6-311++G(d,p). [b]Single point calculation optimised at MP2/6-311++G(d,p). [c]Single point calculation optimised at BHandHLYP/aug-cc-pVDZ. [d]Single point calculation optimised at MP2/aug-cc-pVDZ. [e]Single point calculation optimised at B3LYP/6-31G(d). [f] $\Delta E^{\ddagger}$ for the "forward reactions" calculated at 298 K on B3LYP/6-31G(d) optimised geometry $\Delta E^{\ddagger}$=E[URCCSD(T)/6-31G(d)] – E[ROMP2/6-31G(d)] + E[RO)MP2/G3MP2large] + HLC + SO + TC[B3LYP/6-31G(d)] * 0.9989 + ZPVE[B3LYP/6-31G(d)] * 0.9806. [g] E_{act} for the "forward reactions" calculated at 353 K on B3LYP/6-31G(d) optimised geometry.

Table S2. Calculated activation energies ($\Delta E^{\ddagger}$/kJ mol^{-1}) for the intramolecular homolytic addition reactions of acyl and oxyacyl radicals 1 (Scheme 3).



2 (X = CH_2) **2** (X = O) **3** (X = CH_2) **3** (X = O)

Level of Theory	r_1/ Å	r_2/ Å	r_3/ Å	r_4/ Å
HF/6-31G(d)	2.178	2.217	2.190	2.210
HF/6-311G(d,p)	2.169	2.208	2.182	2.199
B3LYP/6-31G(d)	2.222	2.268	2.213	2.253
BHandHLYP/6-311G(d,p)	2.188	2.221	2.159	2.202
BHandHLYP/6-311++G(d,p)	2.191	2.224	2.157	2.202
BHandHLYP/cc-pVDZ	2.198	2.233	2.173	2.213
BHandHLYP/aug-cc-pVDZ	2.199	2.235	2.159	2.208
BHandHLYP/cc-pVTZ	2.184	2.219	2.150	2.196
BHandHLYP/aug-cc-pVTZ	2.185	2.220	2.149	2.196
MP2/6-311G(d,p)	2.175	2.201	2.103	2.167
MP2/6-311++G(d,p)	2.179	2.206	2.100	2.169
MP2/cc-pVDZ	2.186	2.210	2.119	2.178
MP2/aug-cc-pVDZ	2.177	2.208	2.097	2.172

Figure S1. Calculated lowest energy transition states (2,3) for the cyclization of radicals 1.

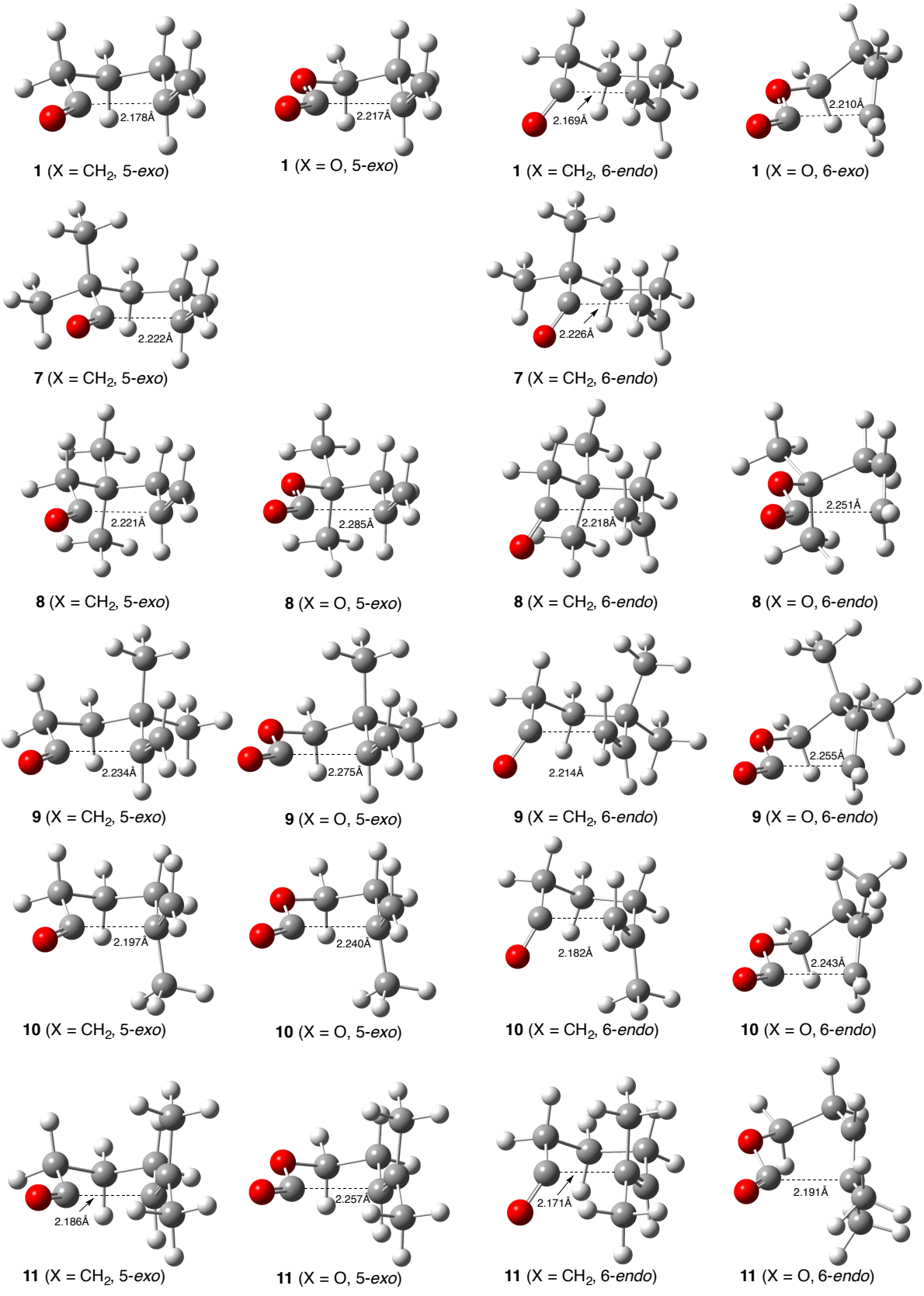
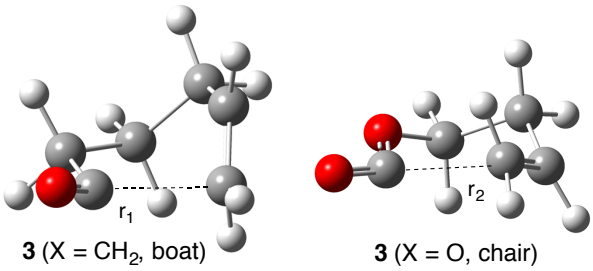


Figure S2. B3LYP/6-31G(d) calculated lowest energy transition states for the cyclization of radicals 1, 7 – 11.



3 (X = CH_2, boat) **3** (X = O, chair)

Level of Theory	r_1 / Å	r_2 / Å
HF/6-31G(d)	2.169	2.202
HF/6-311G(d,p)	2.158	2.191
B3LYP/6-31G(d)	2.207	2.190
BHandHLYP/6-311G(d,p)	2.148	2.182
BHandHLYP/6-311++G(d,p)	2.147	2.183
BHandHLYP/cc-pVDZ	2.158	2.189
BHandHLYP/aug-cc-pVDZ	2.150	2.185
BHandHLYP/cc-pVTZ	2.139	2.177
BHandHLYP/aug-cc-pVTZ	2.139	2.177
MP2/6-311G(d,p)	2.110	2.146
MP2/6-311++G(d,p)	2.108	2.151
MP2/cc-pVDZ	2.120	2.156
MP2/aug-cc-pVDZ	2.109	2.148

Figure S3. Calculated higher energy endo transition states (3) for the cyclization of radicals 1.

B3LYP/6-31G(d) Gaussian Archive Entries for the transition states involved in the cyclization of radicals 1, 7 – 11

Transition state for the cyclization of 1 X=CH2 exo Chair

1\1\GINC-V1436\FTS\UB3LYP\Gen\C6H9O1(2)\AXH563\08-Jan-2013\0\\#B3LYP/g
en 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2
/17=4) Freq=noraman maxdisk=5368709120\\T49.freq\\0,2\C,-0.1185598853,
0.0686699201,0.0208800687\C,-0.0032223026,-0.0070663193,2.2388993393\C
,1.514543722,0.0319426367,2.2124108726\C,2.0632591857,0.7233645694,0.9
495025463\C,-0.6986472273,-1.1185924067,2.6399698798\O,-1.0353795377,-
0.1738349628,-0.6971551403\H,1.8865773749,0.5501727452,3.1063105602\H,
1.8976778951,-0.9963400044,2.2635356071\H,1.8492674795,1.799459482,0.9
952425214\H,3.1514261289,0.6162526273,0.8865931302\H,-0.4992070561,0.9
599634051,2.3285593284\H,-1.7694968963,-1.0865488861,2.8149210094\H,-0
.2203656657,-2.0935068799,2.6982289716\C,1.3712884153,0.1256908391,-0.
2767047829\H,1.5335668557,0.6939453247,-1.2005313333\H,1.7061072837,-0
.9058699744,-0.4616540161\\Version=EM64L-G09RevA.02\State=2-A\HF=-309.
1871969\S2=0.778104\S2-1=0.\S2A=0.750137\RMSD=7.873e-09\RMSF=4.475e-05
\Dipole=0.9899936,0.2111591,0.2047353\Quadrupole=-0.5788347,2.0286392,
-1.4498045,-0.4689301,-2.886031,-0.1866743\PG=C01 [X(C6H9O1)]\\@

Transition state for the cyclization of 10 X=CH2 exo Chair

1\1\GINC-V1422\FTS\UB3LYP\Gen\C7H11O1(2)\AXH563\08-Jan-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=4026531840\\T50.freq\\0,2\C,0.0124307065,
0.000594152,-0.0083276455\C,-0.0229173805,0.0638153142,2.1891563183\C,
1.5023989997,0.060143814,2.2703127721\C,2.1737149165,0.6013332807,0.99
14218432\C,-0.7092540812,-1.0840007876,2.515148766\O,-0.8785464211,-0.
2336633197,-0.7625377287\H,1.8251025445,0.6535192892,3.1366871383\H,1.
8469741863,-0.9669442677,2.4460242952\H,2.0375995811,1.6880456925,0.92
28566469\H,3.2530772029,0.4172460074,1.0150796063\H,-1.791785333,-1.08
94220775,2.6066053316\H,-0.2058905124,-2.0440843142,2.591357966\C,1.51
77115169,-0.0662644615,-0.2176722718\H,1.7682519951,0.4028587745,-1.17
65525559\H,1.7946091393,-1.1286053529,-0.2879627768\C,-0.7080183547,1.
4117497884,2.3540602049\H,-1.7615892885,1.3552195446,2.0639195236\H,-0
.6631987096,1.7319715931,3.4047488621\H,-0.2370210094,2.195250272,1.75
09336829\\Version=EM64L-G09RevA.02\State=2-A\HF=-348.502622\S2=0.77842
3\S2-1=0.\S2A=0.75014\RMSD=6.985e-09\RMSF=1.790e-06\Dipole=0.9412897,0
.1914862,0.303787\Quadrupole=0.3390233,1.5815268,-1.9205502,-0.8719876
,-3.105757,-0.2617748\PG=C01 [X(C7H11O1)]\\@

Transition state for the cyclization of 9 X=CH2 exo Chair

1\1\GINC-V1487\FTS\UB3LYP\Gen\C8H13O1(2)\AXH563\19-Nov-2012\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=2684354560\\T52.freq\\0,2\C,-0.1320874502
,-0.0113083813,0.0063515022\C,0.0232514508,-0.022487716,2.2344864797\C
,1.5560529294,-0.0432960885,2.2050176132\C,2.0359200325,0.7051095361,0
.9309534432\C,-0.7663662883,-1.0417405612,2.6988838175\O,-1.0386695554
,-0.3238474922,-0.6968143758\H,1.7892070573,1.7706059771,1.0339799091\
H,3.1264508208,0.6400243093,0.8399303085\H,-0.3972974817,0.9838086265,

2.2802530625\H,-1.8263897107,-0.8861558138,2.8742884836\H,-0.4045132672,-2.0600199734,2.7987440972\C,1.3432810762,0.1589255155,-0.317990898\H,1.4395276655,0.8187386612,-1.1893044746\H,1.7335837608,-0.8243798521,-0.6148265966\C,2.0771232631,0.7137052164,3.446031095\H,1.7661896208,0.2102517851,4.3676466773\H,3.1733220542,0.7672932013,3.4373173799\H,1.6913839587,1.7397750314,3.4764567315\C,2.1205701047,-1.4764457391,2.2237963256\H,3.2139102118,-1.454416086,2.1453299925\H,1.8667911304,-1.9869886431,3.1584667341\H,1.7357885758,-2.0884267062,1.4002639374\\Version=EM64L-G09RevA.02\State=2-A\HF=-387.8128094\S2=0.777744\S2-1=0.\S2A=0.750135\RMSD=3.599e-09\RMSF=1.273e-05\Dipole=0.9811408,0.246342,0.2021824\Quadrupole=-1.5545387,2.4893548,-0.9348161,-0.7310822,-3.7812536,-0.9236818\PG=C01 [X(C8H13O1)]\\@

Transition state for the cyclization of 8 X=CH2 exo Chair

1\1\GINC-V1487\FTS\UB3LYP\Gen\C8H13O1(2)\AXH563\19-Nov-2012\0\\#B3LYP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=2684354560\\T51.freq\\0,2\C,-0.1894953458,0.1176851838,0.0406058864\C,-0.0151199087,-0.0236374228,2.2499933429\C,1.4995684478,0.0393120396,2.18071309\C,2.0568587047,0.7272562176,0.9031842751\C,-0.674325637,-1.1679991693,2.6165878007\O,-1.1293656752,-0.1020693902,-0.65502221\H,1.8886269573,0.5657458677,3.0640106929\H,1.8929189244,-0.9853335259,2.2311881072\H,-0.534445704,0.9227214686,2.3950072417\H,-1.7411404279,-1.1694973196,2.8176434833\H,-0.1719274312,-2.1325252602,2.6246581167\C,1.2938836163,0.1147272857,-0.2844779134\H,1.4599070587,0.6502194973,-1.2281693069\H,1.5881384115,-0.9333557553,-0.445594124\C,1.8006692702,2.2459117514,0.9516731187\H,2.2917447242,2.6967756608,1.8221598792\H,2.1930072004,2.7377819085,0.0531571062\H,0.7305208953,2.4760407439,1.0131476706\C,3.5646431076,0.4635286665,0.7794112537\H,3.9791182288,0.9367955167,-0.1190050176\H,4.1032840171,0.8665207524,1.6457424156\H,3.7785345136,-0.6108256021,0.7226352538\\Version=EM64L-G09RevA.02\State=2-A\HF=-387.8159058\S2=0.777427\S2-1=0.\S2A=0.750134\RMSD=4.473e-09\RMSF=5.513e-06\Dipole=1.0061091,0.2082392,0.2019114\Quadrupole=-2.0875476,2.5176211,-0.4300735,-0.987076,-3.0445094,-0.1251824\PG=C01 [X(C8H13O1)]\\@

Transition state for the cyclization of 7 X=CH2 exo Chair

1\1\GINC-V1393\FTS\UB3LYP\Gen\C8H13O1(2)\AXH563\01-May-2013\0\\#B3LYP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=1342177280\\T56.freq\\0,2\C,0.0213818462,-0.1073316973,-0.0047102923\C,-0.0326228288,0.0179888901,2.2131097948\C,1.4821949168,-0.0118294891,2.2990792393\C,2.1575211266,0.5093696338,1.0153966801\C,-0.8124281899,-1.0140828394,2.6659626213\O,-0.8528310554,-0.3882905178,-0.7618310054\H,1.8131162154,0.5975274129,3.1509210192\H,1.8085105483,-1.0377964934,2.5104674723\H,-0.4839562218,1.0094028393,2.1648766426\H,-1.8903295438,-0.9175680882,2.7510611881\H,-0.3908091523,-1.9972270714,2.8619481464\C,1.5423360893,-0.1451948034,-0.2348293305\H,2.0097967207,1.5962369331,0.9490013581\H,3.2406747703,0.3398548844,1.0501561601\C,1.8672852048,0.6341277611,-1.5209353058\H,2.948843321,0.6290639465,-1.701900635\H,1.3683661743,0.1827853744,-2.38437945\H,1.5425029525,1.6780883693,-1.4471973596\C,1.954296599,-1.625534633,-0.3860665729\H,1.4596623691,-2.0739591519,-1.2535067081\H,3.0394590025,-1.6950684815,-0.5298856143\H,1.6903947994,-2.2188353731,0.4949898216\\Version=EM64L-G09RevA.02\State=2-A\HF=-387.8165033\S2=0.777261\S2-1=0.

\S2A=0.750133\RMSD=8.080e-09\RMSF=1.000e-06\Dipole=0.9902241,0.1572744
,0.163331\Quadrupole=-1.2533445,2.1806647,-0.9273202,-0.6321124,-2.043
0258,-0.1094868\PG=C01 [X(C8H13O1)]\\@

Transition state for the cyclization of 11 X=CH2 exo Chair

1\1\GINC-V1487\FTS\UB3LYP\Gen\C8H13O1(2)\AXH563\19-Nov-2012\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=2684354560\\T53.freq\\0,2\C,-0.0909452925
,-0.0308096707,0.1042385404\C,0.0431791549,0.0120427735,2.2855371079\C
,1.5578106244,0.116976143,2.2675224199\C,2.0606248174,0.7875824144,0.9
724230368\C,-0.6932511269,-1.0936557527,2.6647345188\O,-0.9624934007,-
0.5187212407,-0.551328355\H,1.7828579952,1.8498435979,0.9767632372\H,3
.1530100522,0.7410090758,0.90656792\H,-0.4657960992,0.9719011651,2.380
0364847\C,1.3934267113,0.1003939249,-0.2189687244\H,1.4960044332,0.657
0114047,-1.1583884912\H,1.8002901785,-0.9076024735,-0.3906023086\H,1.8
966965389,0.6951174419,3.1376095828\H,2.0149346064,-0.8748710575,2.355
8521035\C,-0.160194569,-2.4991501167,2.7226235665\H,0.9281251564,-2.56
06388398,2.6428953216\H,-0.4533229757,-2.9891144946,3.6617501956\H,-0.
5874475426,-3.1099975816,1.9112888492\C,-2.1852440236,-0.9737504598,2.
8153915747\H,-2.6980293868,-1.4118550064,1.9443648567\H,-2.5471871948,
-1.5153605305,3.7004546864\H,-2.5082268423,0.0692516492,2.89531052\\Ve
rsion=EM64L-G09RevA.02\State=2-A\HF=-387.8241486\S2=0.776555\S2-1=0.\S
2A=0.750132\RMSD=6.576e-09\RMSF=5.908e-06\Dipole=0.8058305,0.1439439,0
.4060022\Quadrupole=0.3390878,1.7311881,-2.0702759,0.4701601,-3.471911
9,-1.0848356\PG=C01 [X(C8H13O1)]\\@

Transition state for the cyclization of 1 X=CH2 endo Chair

1\1\GINC-GOMBERG19\FTS\UB3LYP\6-31G(d)\C6H9O1(2)\CARLHS\06-Jan-2014\1\
\#b3lyp/6-31g* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoi
nt guess=read\\Acyl radical endo transition state\\0,2\C\O,1,B1\C,1,B2
,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,B6,
3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,0\C
,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,1,B1
3,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=1.19
691528\B3=1.08615579\B4=1.08770974\B5=1.36452349\B6=1.08900478\B7=1.50
081579\B8=1.09650078\B9=1.09914172\B10=1.54927728\B11=1.09905979\B12=1
.09719468\B13=1.53295419\B14=1.09704773\B15=1.09716358\A1=119.79222894
\A2=101.04221928\A3=92.39269816\A4=92.13928553\A5=119.16224233\A6=121.
13862136\A7=111.76178319\A8=110.44852264\A9=109.1556884\A10=109.980475
72\A11=109.72856086\A12=126.46476507\A13=108.70181607\A14=107.05595908
\D1=-32.34063357\D2=-149.10635956\D3=90.09641738\D4=-93.52100938\D5=69
.26200698\D6=-199.5076152\D7=41.11971647\D8=-78.37444894\D9=-181.97509
118\D10=-64.43621445\D11=138.4952982\D12=150.2829028\D13=33.52788908\B
2=2.21339263\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.1858404\S2=0.
769808\S2-1=0.\S2A=0.750093\RMSD=4.744e-09\RMSF=4.213e-05\Dipole=-0.13
9227,-0.4580079,-0.9011849\Quadrupole=1.6757448,1.2237332,-2.899478,0.
41757,1.6809143,-1.9497734\PG=C01 [X(C6H9O1)]\\@

Transition state for the cyclization of 7 X=CH2 endo Chair

1\1\GINC-GOMBERG01\FTS\UB3LYP\6-31G(d)\C8H13O1(2)\CARLHS\10-Jan-2014\1
\\#b3lyp/6-31g* opt=(grad,ts,readfc,nofreeze,noeigentest) geom=checkpo
int guess=read\\2,2-dimethyl acyl radical endo transition state\\0,2\C

\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,
2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9
,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,
6,D10,0\C,1,B13,2,A12,3,D11,0\C,14,B14,1,A13,2,D12,0\C,14,B15,1,A14,2,
D13,0\H,15,B16,14,A15,11,D14,0\H,15,B17,14,A16,11,D15,0\H,15,B18,14,A1
7,11,D16,0\H,16,B19,14,A18,11,D17,0\H,16,B20,14,A19,11,D18,0\H,16,B21,
14,A20,11,D19,0\\B1=1.19618529\B3=1.08633951\B4=1.08669677\B5=1.363672
89\B6=1.08927241\B7=1.50032604\B8=1.09681866\B9=1.09733535\B10=1.54888
346\B11=1.10049778\B12=1.0979419\B13=1.55796129\B14=1.5404673\B15=1.54
224212\B16=1.09564391\B17=1.09650537\B18=1.09358229\B19=1.0950107\B20=
1.09379064\B21=1.0965909\A1=117.23861627\A2=100.20061188\A3=93.2212432
\A4=91.95374079\A5=119.16422372\A6=120.88779972\A7=111.72278953\A8=110
.74284655\A9=108.85994414\A10=109.77787001\A11=108.56021669\A12=126.17
379856\A13=108.68955437\A14=107.88026094\A15=110.78993949\A16=110.1485
8035\A17=112.43338013\A18=111.0859061\A19=110.94538553\A20=110.1465208
\D1=-26.26923585\D2=-142.93607753\D3=95.95831417\D4=-92.90335755\D5=68
.53561271\D6=-200.09034965\D7=40.85202286\D8=-80.12835668\D9=-179.7328
8208\D10=-63.57422512\D11=143.16626681\D12=140.2955381\D13=21.3078344\
D14=178.44138445\D15=59.22692703\D16=-61.11610328\D17=180.35004654\D18
=60.51842603\D19=-59.84557259\B2=2.22625822\\Version=AM64L-G09RevC.01\
State=2-A\HF=-387.8125945\S2=0.77072\S2-1=0.\S2A=0.750098\RMSD=5.398e-
09\RMSF=4.663e-05\Dipole=-0.2041654,-0.3658983,-0.8649671\Quadrupole=1
.3524092,1.6966421,-3.0490514,-0.160347,0.6320427,-1.6182556\PG=C01 [X
(C8H13O1)]\\@

Transition state for the cyclization of 8 X=CH2 endo Chair

1\1\GINC-GOMBERG19\FTS\UB3LYP\6-31G(d)\C8H13O1(2)\CARLHS\10-Jan-2014\1
\\#b3lyp/6-31g* opt=(grad,ts,readfc,nofreeze,noeigentest) geom=checkpo
int guess=read\\3,3-dimethyl acyl radical endo transition state\\0,2\C
\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,
2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9
,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\C,11,B11,8,A10,6,D9,0\C,11,B12,8,A11,
6,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,
D13,0\H,12,B16,11,A15,14,D14,0\H,12,B17,11,A16,14,D15,0\H,12,B18,11,A1
7,14,D16,0\H,13,B19,11,A18,14,D17,0\H,13,B20,11,A19,14,D18,0\H,13,B21,
11,A20,14,D19,0\\B1=1.19785825\B3=1.08612214\B4=1.0876827\B5=1.3636067
8\B6=1.08830432\B7=1.49941309\B8=1.09741636\B9=1.09938947\B10=1.564835
86\B11=1.54035265\B12=1.53943856\B13=1.53019461\B14=1.09708431\B15=1.0
9813989\B16=1.09674848\B17=1.0968875\B18=1.09649108\B19=1.09673187\B20
=1.09642421\B21=1.09362595\A1=119.68952256\A2=101.65416358\A3=91.88100
592\A4=91.40116949\A5=119.0587246\A6=121.17796325\A7=111.54721502\A8=1
09.96319128\A9=111.43754676\A10=108.9857777\A11=110.87894189\A12=126.8
5020169\A13=108.39084281\A14=106.80251088\A15=110.61646064\A16=111.378
05155\A17=111.17356532\A18=110.47170607\A19=110.68427473\A20=112.09562
757\D1=-32.65492134\D2=-149.41578496\D3=89.76371501\D4=-95.15673424\D5
=69.3867157\D6=-200.75753707\D7=40.54065929\D8=-79.18855364\D9=-187.25
021369\D10=-66.78992044\D11=138.19191856\D12=151.63756934\D13=35.47652
112\D14=178.89499117\D15=58.98687812\D16=-61.50754618\D17=181.20402801
\D18=61.98864891\D19=-57.97543317\B2=2.21819856\\Version=AM64L-G09RevC
.01\State=2-A\HF=-387.813924\S2=0.768886\S2-1=0.\S2A=0.750088\RMSD=7.7
66e-09\RMSF=3.803e-05\Dipole=-0.1467607,-0.4911785,-0.8787791\Quadrupo
le=2.0172505,0.7885574,-2.805808,0.05588,1.0042178,-2.8642117\PG=C01 [
X(C8H13O1)]\\@

Transition state for the cyclization of 9 X=CH2 endo Chair

1\1\GINC-GOMBERG19\FTS\UB3LYP\6-31G(d)\C8H13O1(2)\CARLHS\10-Jan-2014\1
\\#b3lyp/6-31g* opt=(grad,ts,readfc,nofreeze,noeigentest) geom=checkpo
int guess=read\\4,4-dimethyl acyl radical endo transition state\\0,2\C
\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,
2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\C,8,B8,6,A7,3,D6,0\C,8,B9
,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,
6,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,
D13,0\H,9,B16,8,A15,11,D14,0\H,9,B17,8,A16,11,D15,0\H,9,B18,8,A17,11,D
16,0\H,10,B19,8,A18,11,D17,0\H,10,B20,8,A19,11,D18,0\H,10,B21,8,A20,11
,D19,0\\B1=1.19693327\B3=1.08618012\B4=1.08584406\B5=1.36358508\B6=1.0
899107\B7=1.51534802\B8=1.54119746\B9=1.54221918\B10=1.56294567\B11=1.
10049002\B12=1.09753585\B13=1.53315614\B14=1.09542699\B15=1.09728556\B
16=1.09605742\B17=1.09647722\B18=1.09678422\B19=1.09541762\B20=1.09445
949\B21=1.09662924\A1=119.7183681\A2=100.44514664\A3=92.77501545\A4=92
.12727426\A5=118.20844377\A6=123.86998057\A7=110.00451385\A8=112.78375
592\A9=106.1312143\A10=109.22357331\A11=108.82226861\A12=126.36816679\
A13=108.73487025\A14=107.00943511\A15=110.92551007\A16=111.05995164\A1
7=111.1552599\A18=110.52549802\A19=112.92743019\A20=110.28698983\D1=-3
0.76001479\D2=-147.15897841\D3=90.79993166\D4=-92.86959597\D5=70.42123
339\D6=-193.9753455\D7=44.44866651\D8=-76.79095143\D9=-183.23124922\D1
0=-67.04646173\D11=138.10347296\D12=148.34786598\D13=32.00820874\D14=1
79.70113042\D15=59.75049222\D16=-60.31783279\D17=179.68848328\D18=59.2
2124353\D19=-60.96169677\B2=2.21386922\\Version=AM64L-G09RevC.01\State
=2-A\HF=-387.8114356\S2=0.769501\S2-1=0.\S2A=0.750091\RMSD=4.989e-09\R
MSF=1.717e-05\Dipole=-0.10143,-0.467151,-0.9387455\Quadrupole=2.659767
9,1.0907465,-3.7505144,0.4913335,1.6706483,-2.9611701\PG=C01 [X(C8H13O
1)]\\@

Transition state for the cyclization of 10 X=CH2 endo Chair

1\1\GINC-GOMBERG19\FTS\UB3LYP\6-31G(d)\C7H11O1(2)\CARLHS\09-Jan-2014\1
\\#b3lyp/6-31g* opt=(grad,ts,readfc,nofreeze,noeigentest) geom=checkpo
int guess=read\\5_Methyl acyl radical endo transition state\\0,2\C\O,1
,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3
,0\C,6,B6,3,A5,1,D4,0\H,7,B7,6,A6,3,D5,0\H,7,B8,6,A7,3,D6,0\C,7,B9,6,A
8,3,D7,0\H,10,B10,7,A9,6,D8,0\H,10,B11,7,A10,6,D9,0\C,1,B12,2,A11,3,D1
0,0\H,13,B13,1,A12,2,D11,0\H,13,B14,1,A13,2,D12,0\C,6,B15,3,A14,1,D13,
0\H,16,B16,6,A15,3,D14,0\H,16,B17,6,A16,3,D15,0\H,16,B18,6,A17,3,D16,0
\\B1=1.20068798\B3=1.08662538\B4=1.08703333\B5=1.36863989\B6=1.5091796
\B7=1.09696276\B8=1.09843062\B9=1.55040394\B10=1.09864899\B11=1.097036
55\B12=1.53405802\B13=1.09665938\B14=1.09699828\B15=1.50307495\B16=1.0
9765217\B17=1.09410321\B18=1.10149341\A1=118.4107608\A2=101.10220657\A
3=94.17924268\A4=90.72735968\A5=118.54947834\A6=111.52443315\A7=110.29
675439\A8=109.70673845\A9=109.89065795\A10=109.90588262\A11=125.538076
42\A12=109.21798996\A13=107.02244693\A14=121.38313424\A15=111.32316929
\A16=111.64672152\A17=111.14606299\D1=-41.65734983\D2=-158.96670319\D3
=80.11242714\D4=72.49543076\D5=-200.00465701\D6=40.89248105\D7=-78.718
01565\D8=-183.6538286\D9=-66.15278246\D10=133.21968363\D11=158.1141015
6\D12=41.1354355\D13=-91.39232743\D14=-141.85415924\D15=-20.60472395\D
16=98.95408171\B2=2.18185683\\Version=AM64L-G09RevC.01\State=2-A\HF=-3
48.505934\S2=0.767772\S2-1=0.\S2A=0.750082\RMSD=7.373e-09\RMSF=3.842e-
05\Dipole=0.0337461,-0.593028,-0.8518061\Quadrupole=1.7633391,0.361807
9,-2.125147,0.7978952,2.3511563,-2.0936043\PG=C01 [X(C7H11O1)]\\@

Transition state for the cyclization of 11 X=CH2 endo Chair

1\1\GINC-MERRI028\FTS\UB3LYP\6-31G(d)\C8H13O1(2)\ROOT\24-Jan-2014\0\\#
 B3LYP/6-31G(d) Opt=(ts,calcfc,noeigentest) freq=noraman\\g3 6-6-acyl
Chair endo\\0,2\C,0.004053859,-0.3390825176,-0.0089376079\O,-0.2155564
575,-1.3856312376,0.5360428207\C,1.8944820254,-0.1180107524,-1.0523095
827\C,1.2398827823,-0.4207346515,-2.2302681753\H,1.2072253386,-1.46957
99889,-2.5249677705\C,0.2471243414,0.4762982672,-2.9086852319\H,0.1493
891429,0.2194417003,-3.9706459553\H,0.5471721548,1.5303626588,-2.86396
64185\C,-1.1276121817,0.3056766128,-2.2148312284\H,-1.4939845451,-0.71
54881086,-2.3798938128\H,-1.8670229939,0.9894977396,-2.6550870762\C,2.
255229411,1.2998616094,-0.6464052788\H,2.2981998677,1.3941148814,0.443
3747585\H,3.251468429,1.5503857054,-1.0382601764\H,1.5564410514,2.0497
296245,-1.0240798433\C,2.7509141497,-1.1797373264,-0.395081972\H,3.810
8395986,-1.0176464889,-0.6335451296\H,2.6467451108,-1.1456085154,0.694
4644257\H,2.4731862741,-2.1843473239,-0.7263110423\C,-1.0324529302,0.5
591344057,-0.6967113107\H,-0.7668085441,1.6074852508,-0.5150448173\H,-
1.9981381715,0.3642830719,-0.2141061822\\Version=AM64L-G09RevC.01\Stat
e=2-A\HF=-387.8188133\S2=0.771886\S2-1=0.\S2A=0.750106\RMSD=4.252e-09\
RMSF=2.002e-05\Dipole=0.023071,0.7387098,-0.629917\Quadrupole=1.981238
5,-0.5260679,-1.4551705,-1.6492301,2.0711678,2.5845205\PG=C01 [X(C8H13
O1)]\\@

Transition state for the cyclization of 1 X=O exo Chair

1\1\GINC-V1468\FTS\UB3LYP\Gen\C5H7O2(2)\AXH563\24-Jun-2012\0\\#B3LYP/g
en 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2
/17=4) Freq=noraman maxdisk=5368709120\\A23-TS.freq\\0,2\C,-0.02675916
58,0.0465214952,-0.0269608214\C,-0.0071129307,-0.0026014619,2.24005664
28\C,1.503494965,0.0029673903,2.1666167351\C,1.9860721668,0.7306750078
,0.9122520671\O,1.2891157034,0.2302685793,-0.2498817943\C,-0.723976471
5,-1.0953886302,2.6340807601\O,-0.8328135721,-0.2987771093,-0.83203565
34\H,1.9340388644,0.5005608956,3.0465427766\H,1.8751626312,-1.02857276
94,2.1602892986\H,1.8104550185,1.8109536003,0.9833689163\H,3.045765523
6,0.5604289076,0.713062194\H,-0.4855059241,0.9748753921,2.3015114623\H
,-1.7925575757,-1.0368456831,2.8144817414\H,-0.2669667075,-2.079805207
6,2.6963700072\\Version=EM64L-G09RevA.02\State=2-A\HF=-345.0989824\S2=
0.779036\S2-1=0.\S2A=0.750154\RMSD=5.438e-09\RMSF=2.605e-06\Dipole=0.9
035527,0.3964689,1.1493192\Quadrupole=1.3412789,2.4542162,-3.7954952,0
.2174307,-1.6505652,-0.4971918\PG=C01 [X(C5H7O2)]\\@

Transition state for the cyclization of 8 X=O exo Chair

1\1\GINC-V1311\FTS\UB3LYP\Gen\C7H11O2(2)\AXH563\01-May-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=1342177280\\T29-2.freq\\0,2\C,-0.01996692
03,0.0334949648,0.0004807146\C,-0.0254383802,-0.018087663,2.2846269857
\C,1.4830089763,0.0435084677,2.2209570574\C,2.0171608631,0.7457733788,
0.9540193788\O,1.296668162,0.1969805555,-0.200858067\C,-0.6959851337,-
1.1430328004,2.6614759317\O,-0.8173688164,-0.3355996333,-0.804715632\H
,1.8812353056,0.5733740891,3.0973226565\H,1.8825843907,-0.9773491342,2
.2551752272\H,-0.5535982107,0.9321243321,2.3419056461\H,-1.7679757616,
-1.1335591628,2.8314230508\H,-0.1962482638,-2.1064603878,2.726556934\C
,1.7915559392,2.2603108914,0.9764277923\H,2.3698979281,2.7212211648,1.

7848246727\H,2.1096039564,2.7031956335,0.0273180901\H,0.7349661604,2.5
047789068,1.1268558539\C,3.4828084186,0.4040961567,0.700795094\H,3.843
6591871,0.8911218057,-0.2106300422\H,4.0982652152,0.7437142253,1.54096
76777\H,3.6120545674,-0.6769975052,0.5893864449\\Version=EM64L-G09RevA
.02\State=2-A\HF=-423.7358095\S2=0.777528\S2-1=0.\S2A=0.750144\RMSD=3.
663e-09\RMSF=1.891e-05\Dipole=1.0208059,0.5217562,1.0778077\Quadrupole
=0.3389521,2.67969,-3.018642,-0.6359975,-2.8982419,-1.3818396\PG=C01 [
X(C7H11O2)]\\@

Transition state for the cyclization of 9 X=O exo Chair

1\1\GINC-V1448\FTS\UB3LYP\Gen\C7H11O2(2)\AXH563\01-May-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=1342177280\\T30-2.freq\\0,2\C,-0.01992855
71,-0.0443060121,-0.0038802166\C,0.0122725948,-0.0125131855,2.27082846
49\C,1.5385078345,-0.0461932721,2.2195105454\C,1.9633764091,0.70035947
02,0.9409561081\O,1.2921728874,0.1679388872,-0.2214807256\C,-0.7884171
935,-1.0274446561,2.7075865196\O,-0.8119918987,-0.4257309909,-0.806359
533\H,1.7317625162,1.7702338006,1.0150105158\H,3.0303845976,0.58500810
13,0.7372535269\H,-0.4083078299,0.9942178558,2.2855123961\H,-1.8495575
699,-0.8655104369,2.8687208963\H,-0.4309192035,-2.0459817208,2.8179417
394\C,2.1087132313,0.7219063305,3.431097712\H,1.8502036913,0.208963141
,4.3627891809\H,3.2024428751,0.7901197054,3.3726392631\H,1.7083113104,
1.7410764478,3.4862731207\C,2.1014186804,-1.4777256252,2.1967674987\H,
3.1956519777,-1.4525746681,2.1378397894\H,1.8322734393,-2.0211613196,3
.1078837446\H,1.7299438045,-2.0451278739,1.3374359877\\Version=EM64L-G
09RevA.02\State=2-A\HF=-423.72658\S2=0.778224\S2-1=0.\S2A=0.75015\RMSD
=7.033e-09\RMSF=1.029e-05\Dipole=0.9035272,0.3878876,1.1881217\Quadrup
ole=0.9325244,3.4332399,-4.3657643,-0.1485792,-3.0843265,-1.030248\PG=
C01 [X(C7H11O2)]\\@

Transition state for the cyclization of 10 X=O exo Chair

1\1\GINC-V1437\FTS\UB3LYP\Gen\C6H9O2(2)\AXH563\01-May-2013\0\\#B3LYP/g
en 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2
/17=4) Freq=noraman maxdisk=1342177280\\T32-2.freq\\0,2\C,0.0376140512
,-0.0366113788,-0.0101383257\C,-0.0355139898,0.0568561772,2.2267692739
\C,1.485584972,0.0409282125,2.219523241\C,2.047009379,0.6476419655,0.9
321785038\O,1.3660501958,0.0871437267,-0.2101751843\C,-0.7152996097,-1
.0836732254,2.5723202997\O,-0.7575893843,-0.4047941518,-0.8169278537\H
,1.8819364503,0.60379757,3.0762319614\H,1.8406828074,-0.9912675773,2.3
135240015\H,1.9287630178,1.7370689022,0.9070339125\H,3.1031149282,0.40
95260649,0.7918329525\H,-1.792163823,-1.0782894004,2.7132847566\H,-0.2
174391065,-2.0478546275,2.6240312426\C,-0.7086242553,1.4102356103,2.38
82692464\H,-1.7802455602,1.3414048409,2.1803331541\H,-0.5863912938,1.7
698566672,3.4194144657\H,-0.2895189865,2.1720086505,1.7229312104\\Vers
ion=EM64L-G09RevA.02\State=2-A\HF=-384.4145419\S2=0.780463\S2-1=0.\S2A
=0.750163\RMSD=4.626e-09\RMSF=4.844e-06\Dipole=0.8203976,0.496025,1.19
74656\Quadrupole=2.2715625,2.0370535,-4.3086159,-0.1595241,-1.5319126,
-1.1795963\PG=C01 [X(C6H9O2)]\\@

Transition state for the cyclization of 10 X=O exo Chair

1\1\GINC-V1469\FTS\UB3LYP\Gen\C7H11O2(2)\AXH563\01-May-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(

2/17=4) Freq=noraman maxdisk=1342177280\\T31-2.freq\\0,2\C,0.0510898767,-0.0633086644,0.0500855303\C,0.0491903536,-0.014208621,2.3068862806\C,1.5579215868,0.075794685,2.2631481424\C,2.0050039327,0.770127832,0.974021959\O,1.3716382401,0.1429480668,-0.1599297818\C,-0.7004602635,-1.1057210117,2.6764341126\O,-0.7029694528,-0.5549913349,-0.7332756345\H,1.9369959938,0.6489116573,3.1208215933\H,2.0159454882,-0.9164989169,2.3093874059\H,1.7421483689,1.8351369205,0.9815758285\H,3.0788015723,0.6750301195,0.8009478403\H,-0.4554218046,0.9511780675,2.3499101891\C,-2.1915518319,-0.9709523479,2.8282679064\H,-2.7125403526,-1.492431478,2.0111762759\H,-2.541450562,-1.426566057,3.7651509638\H,-2.5148115439,0.0745316908,2.8135850286\C,-0.1732538907,-2.5103860865,2.7827513863\H,0.9140078779,-2.5805505083,2.7014797917\H,-0.4676766877,-2.9645051521,3.7389908918\H,-0.6064958067,-3.1425495843,1.9930196301\\Version=EM64L-G09RevA.02\State=2-A\HF=-423.7370868\S2=0.776081\S2-1=0.\S2A=0.750137\RMSD=8.933e-09\RMSF=4.396e-06\Dipole=0.6502154,0.2943558,1.3136561\Quadrupole=2.5455705,3.1100916,-5.6556621,1.5594017,-1.4491547,-0.7634087\PG=C01 [X(C7H11O2)]\\@

Transition state for the cyclization of 1 X=O endo Boat

1\1\GINC-V1434\FTS\UB3LYP\Gen\C5H7O2(2)\AXH563\22-May-2012\0\\#B3LYP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=5368709120\\S29.freq\\0,2\C,0.1161432984,0.0484926647,0.050907683\O,0.0096568886,-0.0045485837,1.4020123296\O,1.1513318825,0.0444851084,-0.5428880568\C,-1.7927871023,-0.8468639954,-0.7415494346\H,-1.5386720266,-1.1343548222,-1.7577903238\H,-2.249927513,0.1333990737,-0.6444101777\C,-1.8740999926,-1.7801599393,0.2511755018\H,-1.5580549291,-2.8000038582,0.0456803583\C,-2.0232184852,-1.3714692718,1.6944073445\H,-1.5743631092,-2.1349390755,2.3399754757\H,-3.0742162208,-1.2769121176,2.0080592505\C,-1.3274163721,-0.0217084293,1.9422922844\H,-1.199582802,0.1694398261,3.0097753532\H,-1.8992007711,0.8077098787,1.5135186929\\Version=EM64L-G09RevA.02\State=2-A\HF=-345.0913593\S2=0.776954\S2-1=0.\S2A=0.75014\RMSD=4.543e-09\RMSF=1.432e-05\Dipole=-1.3788205,-0.2222829,0.644562\Quadrupole=-3.8526968,1.9892529,1.8634439,-1.9867501,0.879696,0.682656\PG=C01 [X(C5H7O2)]\\@

Transition state for the cyclization of 8 X=O endo Boat

1\1\GINC-V1440\FTS\UB3LYP\Gen\C7H11O2(2)\AXH563\03-Jan-2013\0\\#B3LYP/gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2/17=4) Freq=noraman maxdisk=2684354560\\S29-2.freq\\0,2\C,-0.0823307049,0.1015280526,-0.0531721336\O,-0.0994277973,0.102246449,1.2994153089\O,0.9125240304,0.2006262402,-0.7090739097\C,-1.7594441552,-1.2367700734,-0.734913584\H,-1.3341754638,-1.6438072689,-1.6479842539\H,-2.425863978,-0.3905877519,-0.8724981173\C,-1.7258422413,-1.9394269988,0.4304644099\H,-1.143633587,-2.8571252077,0.4728055749\C,-2.1233740996,-1.31122484,1.7358520594\H,-1.905404187,-2.0022554698,2.5562282645\H,-3.2029555183,-1.1109584244,1.7752643242\C,-1.3806087835,0.0520218502,2.0049989171\C,-2.2243979975,1.2670550052,1.6043579112\H,-3.1328622001,1.311722749,2.2150340964\H,-1.6542259901,2.1878110614,1.7655309423\H,-2.5232914845,1.2322055069,0.5533775826\C,-0.975257374,0.1469452428,3.4767015659\H,-1.8615757289,0.0696048955,4.1157683931\H,-0.288130114,-0.6643856047,3.7363386079\H,-0.4785897458,1.1002955179,3.6827701408\\Version=EM64L-G09RevA.02\State=2-A\HF=-423.723196\S2=0.775265\S2-1=0.\S2A=0.750131\RMSD=4.105e-09\RMSF=7.586e-06\Dipole=-1.2946596,-0.2158791,0.852813

6\Quadrupole=-3.3302169,2.3914808,0.9387362,-2.1023051,2.6914888,1.124
1626\PG=C01 [X(C7H11O2)]\\@

Transition state for the cyclization of 9 X=O endo Boat

1\1\GINC-V1466\FTS\UB3LYP\Gen\C7H11O2(2)\AXH563\21-May-2012\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=5368709120\\S30.freq\\0,2\C,0.0220882615,
0.2698163394,-0.0373452163\O,-0.0416964126,0.2014963937,1.1524617138\O
,1.0836680397,-0.1428968557,-0.7724572542\C,0.0113540638,-1.06499201,-
2.8195923757\C,0.9626862745,-0.0079202517,-2.2033426354\H,0.6353920205
,1.0092294244,-2.4431621903\H,1.9802820261,-0.135837816,-2.580954902\C
,-0.2325879411,-0.688976771,-4.297443482\H,0.713193853,-0.6392763799,-
4.8527069629\H,-0.8675879017,-1.4372464129,-4.7833076145\H,-0.73294684
41,0.2819033383,-4.3848060025\C,0.663940592,-2.4578851309,-2.728847776
3\H,-0.0182688505,-3.2287664127,-3.1054758125\H,1.5826719065,-2.500939
9021,-3.3257034105\H,0.918803939,-2.7045090781,-1.6927931392\C,-1.2720
070949,-1.0567201271,-2.00927226\H,-1.6685952694,-2.0209981788,-1.6966
479119\C,-1.749884359,0.0757416714,-1.4177171034\H,-1.5198982686,1.065
6666267,-1.8002587499\H,-2.596243824,0.0341915864,-0.7379494593\\Versi
on=EM64L-G09RevA.02\State=2-A\HF=-423.720754\S2=0.776152\S2-1=0.\S2A=0
.750135\RMSD=5.377e-09\RMSF=2.983e-05\Dipole=-0.1453673,-0.1259716,-1.
5416204\Quadrupole=2.4620987,3.2197098,-5.6818085,0.1677569,-2.0418035
,-1.7921839\PG=C01 [X(C7H11O2)]\\@

Transition state for the cyclization of 10 X=O endo Boat

1\1\GINC-MERRI005\FTS\UB3LYP\6-31G(d)\C7H11O2(2)\ROOT\22-Jan-2014\1\\#
 B3LYP/6-31G(d) Opt=(grad,ts,noeigentest) freq=noraman\\g3 6-6-acyl Ch
air endo\\0,2\C\O,1,B1\C,1,B2,2,A1\C,3,B3,1,A2,2,D1,0\H,4,B4,3,A3,1,D2
,0\C,4,B5,3,A4,1,D3,0\H,6,B6,4,A5,3,D4,0\H,6,B7,4,A6,3,D5,0\C,6,B8,4,A
7,3,D6,0\H,9,B9,6,A8,4,D7,0\H,9,B10,6,A9,4,D8,0\C,3,B11,1,A10,2,D9,0\H
,12,B12,3,A11,1,D10,0\H,12,B13,3,A12,1,D11,0\H,12,B14,3,A13,1,D12,0\C,
3,B15,1,A14,2,D13,0\H,16,B16,3,A15,1,D14,0\H,16,B17,3,A16,1,D15,0\H,16
,B18,3,A17,1,D16,0\O,9,B19,6,A18,4,D17,0\\B1=1.19761857\B2=2.19133601\
B3=1.38252085\B4=1.08789984\B5=1.50373765\B6=1.09445752\B7=1.09969131\
B8=1.55281328\B9=1.09189936\B10=1.09350128\B11=1.5135634\B12=1.0978401
9\B13=1.09496684\B14=1.09398225\B15=1.52034913\B16=1.0992393\B17=1.092
02104\B18=1.09438046\B19=1.43886131\A1=119.11353224\A2=89.69806349\A3=
117.25384145\A4=123.20366903\A5=109.1633088\A6=113.13244808\A7=110.801
80874\A8=111.0795635\A9=111.31279091\A10=101.31984905\A11=110.43777228
\A12=110.39221685\A13=111.7864199\A14=100.29885991\A15=108.6220427\A16
=113.5553783\A17=111.35727281\A18=112.71947766\D1=123.94430663\D2=-92.
5932951\D3=66.56542662\D4=-166.71322614\D5=74.86502141\D6=-45.97001048
\D7=-150.75772093\D8=88.78009871\D9=4.00470118\D10=-158.53162709\D11=-
39.3887159\D12=80.61802221\D13=-112.6745728\D14=169.04874904\D15=-71.7
0091466\D16=51.02721142\D17=-33.65734561\\Version=AM64L-G09RevC.01\Sta
te=2-A\HF=-423.7239285\S2=0.7796\S2-1=0.\S2A=0.750155\RMSD=9.228e-09\R
MSF=3.678e-05\Dipole=0.3821336,0.0415469,-1.436431\Quadrupole=0.682961
8,2.0488561,-2.731818,0.3434793,4.3431906,-0.0671389\PG=C01 [X(C7H11O2
)]\\@

Transition state for the cyclization of 11 X=O endo Boat

1\1\GINC-MERRI005\FTS\UB3LYP\6-31G(d)\C7H11O2(2)\ROOT\22-Jan-2014\1\\#

B3LYP/6-31G(d) Opt=(grad,ts,noeigentest) freq=noraman\\g3 6-6-acyl Ch
air endo\\0,2\C\O,1,B1\C,1,B2,2,A1\C,3,B3,1,A2,2,D1,0\H,4,B4,3,A3,1,D2
,0\C,4,B5,3,A4,1,D3,0\H,6,B6,4,A5,3,D4,0\H,6,B7,4,A6,3,D5,0\C,6,B8,4,A
7,3,D6,0\H,9,B9,6,A8,4,D7,0\H,9,B10,6,A9,4,D8,0\C,3,B11,1,A10,2,D9,0\H
,12,B12,3,A11,1,D10,0\H,12,B13,3,A12,1,D11,0\H,12,B14,3,A13,1,D12,0\C,
3,B15,1,A14,2,D13,0\H,16,B16,3,A15,1,D14,0\H,16,B17,3,A16,1,D15,0\H,16
,B18,3,A17,1,D16,0\O,9,B19,6,A18,4,D17,0\\B1=1.19761857\B2=2.19133601\
B3=1.38252085\B4=1.08789984\B5=1.50373765\B6=1.09445752\B7=1.09969131\
B8=1.55281328\B9=1.09189936\B10=1.09350128\B11=1.5135634\B12=1.0978401
9\B13=1.09496684\B14=1.09398225\B15=1.52034913\B16=1.0992393\B17=1.092
02104\B18=1.09438046\B19=1.43886131\A1=119.11353224\A2=89.69806349\A3=
117.25384145\A4=123.20366903\A5=109.1633088\A6=113.13244808\A7=110.801
80874\A8=111.0795635\A9=111.31279091\A10=101.31984905\A11=110.43777228
\A12=110.39221685\A13=111.7864199\A14=100.29885991\A15=108.6220427\A16
=113.5553783\A17=111.35727281\A18=112.71947766\D1=123.94430663\D2=-92.
5932951\D3=66.56542662\D4=-166.71322614\D5=74.86502141\D6=-45.97001048
\D7=-150.75772093\D8=88.78009871\D9=4.00470118\D10=-158.53162709\D11=-
39.3887159\D12=80.61802221\D13=-112.6745728\D14=169.04874904\D15=-71.7
0091466\D16=51.02721142\D17=-33.65734561\\Version=AM64L-G09RevC.01\Sta
te=2-A\HF=-423.7239285\S2=0.7796\S2-1=0.\S2A=0.750155\RMSD=9.228e-09\R
MSF=3.678e-05\Dipole=0.3821336,0.0415469,-1.436431\Quadrupole=0.682961
8,2.0488561,-2.731818,0.3434793,4.3431906,-0.0671389\PG=C01 [X(C7H11O2
)]\\@

Gaussian Archive Entries for transition states 2, 3 at all levels of theory used in this study

Transition State 2 X=CH2 exo Chair

HF/6-31G(d)

1\1\GINC-GOMBERG02\FTS\UHF\6-31G(d)\C6H9O1(2)\AHANCOCK\23-Apr-2013\1\\
#P Geom=AllCheck Guess=Read HF/6-31G* opt=(grad,nofreeze,ts,noeigentes
t,readfc)\\9-1-A Benchmark\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,
0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6
,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,2,B10,1,A9,6,D8,0\H,5,
B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0\C,1,B13,6,A12,2,D11,0\H,14,B14,
1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\B2=1.51617501\B3=1.53479335\B4=1
.39007114\B5=1.16886353\B6=1.08671316\B7=1.08730593\B8=1.08729692\B9=1
.08432658\B10=1.07951819\B11=1.07428046\B12=1.07608769\B13=1.51390991\
B14=1.08472075\B15=1.08794774\A1=92.03898271\A2=111.28960413\A3=108.72
857863\A4=129.84978911\A5=109.98847253\A6=109.25618823\A7=109.50405746
\A8=110.95857294\A9=92.95697906\A10=121.09068746\A11=121.22982208\A12=
130.39564744\A13=109.65560293\A14=106.80459191\D1=29.9821384\D2=-143.6
5235579\D3=44.92761571\D4=151.9470939\D5=-91.15592966\D6=68.72889796\D
7=-173.40442326\D8=-74.63058513\D9=-85.9692058\D10=85.75537292\D11=173
.83088267\D12=39.71814993\D13=-76.77809222\B1=2.17795834\\Version=AM64
L-G09RevC.01\State=2-A\HF=-307.2265835\S2=1.010165\S2-1=0.\S2A=0.76256
6\RMSD=8.183e-09\RMSF=1.726e-05\Dipole=1.0748883,0.1870682,0.463449\Qu
adrupole=-0.4332417,2.5643193,-2.1310776,-0.4704531,-3.6109254,-0.3963
076\PG=C01 [X(C6H9O1)]\\@

HF/6-311G(d,p)

1\1\GINC-GOMBERG03\FTS\UHF\6-311G(d,p)\C6H9O1(2)\AHANCOCK\23-Apr-2013\
1\\#P Geom=AllCheck Guess=Read HF/6-311G** opt=(grad,nofreeze,ts,noeig
entest,readfc)\\9-1-A Benchmark\\0,2\C\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,
1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7
,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,2,B10,1,A9,6,D8,0
\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0\C,1,B13,6,A12,2,D11,0\H,14
,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\B2=1.51580094\B3=1.53410206
\B4=1.38937222\B5=1.16193516\B6=1.08680933\B7=1.08780302\B8=1.08786847
\B9=1.08450389\B10=1.08015048\B11=1.0748522\B12=1.07678554\B13=1.51252
104\B14=1.08485522\B15=1.08838468\A1=92.18299793\A2=111.16449881\A3=10
8.80309661\A4=129.26789213\A5=109.96072076\A6=109.22137888\A7=109.4600
7072\A8=111.01579666\A9=92.82000922\A10=120.98706591\A11=121.14854353\
A12=130.90158905\A13=109.57004962\A14=106.42632008\D1=30.03661156\D2=-
143.81238825\D3=45.33951962\D4=151.96302691\D5=-91.06654153\D6=68.7565
4333\D7=-173.27492358\D8=-74.09897436\D9=-85.68963504\D10=85.98664476\
D11=174.6988097\D12=39.10305763\D13=-77.34356155\B1=2.1693602\\Version
=AM64L-G09RevC.01\State=2-A\HF=-307.3020436\S2=1.000553\S2-1=0.\S2A=0.
761655\RMSD=7.983e-09\RMSF=1.284e-05\Dipole=1.0870243,0.1916444,0.4094
322\Quadrupole=-0.3761531,2.5583882,-2.1822351,-0.4869042,-3.4380686,-
0.3288276\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/6-311G(d,p)

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\6-311G(d,p)\C6H9O1(2)\AHANCOCK\26-Ma
r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/6-311G** freq=noraman

opt=(grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C,1,
B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,
0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8
,2,D7,0\H,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0
\C,1,B13,6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\
B2=1.50861282\B3=1.52879857\B4=1.36278706\B5=1.16797883\B6=1.08737864\
B7=1.08834678\B8=1.08801797\B9=1.08481737\B10=1.08066689\B11=1.0753538
7\B12=1.07748317\B13=1.50643199\B14=1.08611338\B15=1.08961296\A1=91.94
218941\A2=112.05234662\A3=107.31866284\A4=128.98931243\A5=109.54310285
\A6=108.93240876\A7=109.55859379\A8=110.96549987\A9=91.58110108\A10=12
1.35245879\A11=121.12769136\A12=131.06010868\A13=109.18953199\A14=106.
58148628\D1=27.76655235\D2=-142.07761736\D3=42.43298929\D4=149.8166372
4\D5=-93.74447582\D6=69.42381085\D7=-172.57994506\D8=-77.05942064\D9=-
86.69703738\D10=87.178916\D11=166.18148157\D12=42.90721969\D13=-73.216
81694\B1=2.18821132\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.073879
1\S2=0.819239\S2-1=0.\S2A=0.750715\RMSD=8.152e-09\RMSF=1.245e-05\Dipol
e=1.0455244,0.2087475,0.2503696\Quadrupole=-0.2748003,2.275643,-2.0008
427,-0.534439,-2.865135,-0.2273895\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG17\FTS\UBHandHLYP\6-311++G(d,p)\C6H9O1(2)\AHANCOCK\27-
Mar-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/6-311++G** freq=nora
man opt=(grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\
C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5
,D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,
3,A8,2,D7,0\H,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D
10,0\C,1,B13,6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13
,0\\B2=1.50831831\B3=1.52851931\B4=1.36334836\B5=1.16871073\B6=1.08744
813\B7=1.08841881\B8=1.08815487\B9=1.08488843\B10=1.08080447\B11=1.075
42747\B12=1.07754756\B13=1.50417175\B14=1.08631972\B15=1.08978662\A1=9
1.85427328\A2=112.0219477\A3=107.50296069\A4=129.02366406\A5=109.50408
386\A6=108.94978015\A7=109.60985705\A8=110.95307464\A9=91.24295825\A10
=121.34916759\A11=121.12576151\A12=131.21940969\A13=109.25832622\A14=1
06.43434396\D1=28.02784109\D2=-142.30702408\D3=43.18263437\D4=150.0161
7481\D5=-93.57024749\D6=69.41046197\D7=-172.61733553\D8=-76.20108055\D
9=-86.52136256\D10=87.42738482\D11=167.7016106\D12=41.93495517\D13=-74
.15703847\B1=2.19077475\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.07
92098\S2=0.817065\S2-1=0.\S2A=0.750676\RMSD=5.353e-09\RMSF=1.108e-05\D
ipole=1.1299476,0.2293874,0.2910935\Quadrupole=-0.192066,2.4979873,-2.
3059213,-0.5413431,-3.1145787,-0.2224447\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-GOMBERG17\FTS\UBHandHLYP\CC-pVDZ\C6H9O1(2)\AHANCOCK\27-Mar-20
13\1\\#P Geom=AllCheck Guess=Read BHandHLYP/cc-pVDZ freq=noraman opt=(
grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C,1,B1\C,
2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,0\H,3
,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7
,0\H,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0\C,1,
B13,6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\B2=1.
50908839\B3=1.52809157\B4=1.36712296\B5=1.17320041\B6=1.09534476\B7=1.
09626816\B8=1.09628691\B9=1.0926618\B10=1.08884375\B11=1.0837238\B12=1
.08592763\B13=1.50793054\B14=1.0938757\B15=1.09754239\A1=91.80026315\A
2=112.13827027\A3=107.74615907\A4=129.6108264\A5=109.56878462\A6=108.9
2100903\A7=109.59565621\A8=111.02834392\A9=91.0788391\A10=121.25810912
\A11=121.0669136\A12=130.8571499\A13=109.37511876\A14=106.3700726\D1=2

7.66683416\D2=-142.18277175\D3=43.37675299\D4=149.75339711\D5=-93.9151
9711\D6=69.14018995\D7=-172.98534698\D8=-75.95031969\D9=-86.41307101\D
10=87.35177791\D11=167.20548141\D12=41.23783683\D13=-74.75661982\B1=2.
19827352\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.0119613\S2=0.8212
34\S2-1=0.\S2A=0.75074\RMSD=7.767e-09\RMSF=7.469e-06\Dipole=1.0133051,
0.1990057,0.236481\Quadrupole=-0.2726883,2.1476242,-1.8749359,-0.49858
08,-2.7177412,-0.1371362\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\Aug-CC-pVDZ\C6H9O1(2)\AHANCOCK\28-Ma
r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/aug-cc-pVDZ freq=noram
an opt=(grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C
,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,
D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3
,A8,2,D7,0\H,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D1
0,0\C,1,B13,6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,
0\\B2=1.50910088\B3=1.52874244\B4=1.36664306\B5=1.17424265\B6=1.092522
37\B7=1.09314069\B8=1.09285365\B9=1.09001385\B10=1.08623592\B11=1.0810
8297\B12=1.08318346\B13=1.50606001\B14=1.09121327\B15=1.09450931\A1=91
.67560994\A2=112.07374691\A3=107.36409809\A4=129.29628927\A5=109.47219
488\A6=108.90062119\A7=109.60072337\A8=110.83382259\A9=91.07248339\A10
=121.33978386\A11=121.13524236\A12=130.92738608\A13=109.08103594\A14=1
06.42869209\D1=28.32352669\D2=-142.49378758\D3=42.08308824\D4=150.2429
2087\D5=-93.25862775\D6=69.11145548\D7=-172.87012473\D8=-77.23489138\D
9=-86.68306944\D10=87.61873948\D11=166.69512709\D12=42.99454033\D13=-7
3.16754958\B1=2.19936252\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.0
313789\S2=0.817626\S2-1=0.\S2A=0.750706\RMSD=7.641e-09\RMSF=9.998e-06\
Dipole=1.1172707,0.2436605,0.3063121\Quadrupole=-0.156667,2.498523,-2.
341856,-0.5828227,-3.0693641,-0.2575551\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-GOMBERG10\FTS\UBHandHLYP\CC-pVTZ\C6H9O1(2)\AHANCOCK\02-Apr-20
13\1\\#P Geom=AllCheck Guess=Read BHandHLYP/cc-pVTZ freq=noraman opt=(
grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C,1,B1\C,
2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,0\H,3
,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7
,0\H,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0\C,1,
B13,6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\B2=1.
50488176\B3=1.52522642\B4=1.35927562\B5=1.16710331\B6=1.0850995\B7=1.0
8592594\B8=1.08563746\B9=1.08240019\B10=1.0782223\B11=1.07294242\B12=1
.07504919\B13=1.50173412\B14=1.08376904\B15=1.08731917\A1=91.88339483\
A2=112.08856419\A3=107.55943655\A4=129.0485822\A5=109.56213419\A6=108.
91637377\A7=109.59373178\A8=110.95764149\A9=91.23111638\A10=121.389340
18\A11=121.11285924\A12=131.14811219\A13=109.26113896\A14=106.46506022
\D1=27.90636284\D2=-142.24679976\D3=43.05830103\D4=149.93983551\D5=-93
.66901908\D6=69.48544644\D7=-172.563731\D8=-76.36825058\D9=-86.5027666
8\D10=87.46649695\D11=167.40127986\D12=42.01772654\D13=-74.03651634\B1
=2.18407212\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.1052901\S2=0.8
16738\S2-1=0.\S2A=0.750697\RMSD=1.074e-09\RMSF=1.052e-05\Dipole=1.0721
484,0.223065,0.2571132\Quadrupole=-0.2319409,2.3106136,-2.0786727,-0.5
428817,-2.8734725,-0.1819823\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/aug-cc-pVTZ

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\Aug-CC-pVTZ\C6H9O1(2)\AHANCOCK\03-Ap
r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/aug-cc-pVTZ freq=noram

an opt=(grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C
,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,
D3,0\H,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3
,A8,2,D7,0\H,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D1
0,0\C,1,B13,6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,
0\\B2=1.50471699\B3=1.52511966\B4=1.35916445\B5=1.16690416\B6=1.084955
1\B7=1.08580179\B8=1.08552292\B9=1.08228115\B10=1.07825135\B11=1.07290
586\B12=1.07501959\B13=1.50118552\B14=1.08373994\B15=1.08723996\A1=91.
85470914\A2=112.06048289\A3=107.52776446\A4=128.96552174\A5=109.536197
81\A6=108.93000965\A7=109.59899712\A8=110.9509212\A9=91.13262717\A10=1
21.39004189\A11=121.1157417\A12=131.28349033\A13=109.24819534\A14=106.
4085622\D1=28.029181\D2=-142.35575262\D3=43.15765239\D4=150.01872096\D
5=-93.56681329\D6=69.43507992\D7=-172.60360319\D8=-76.22433119\D9=-86.
5095414\D10=87.54197635\D11=167.7733933\D12=41.89316243\D13=-74.173302
43\B1=2.18536073\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.1088615\S
2=0.815456\S2-1=0.\S2A=0.750678\RMSD=8.792e-09\RMSF=1.020e-05\Dipole=1
.1137386,0.2363273,0.2801401\Quadrupole=-0.1682007,2.4504774,-2.282276
7,-0.5552906,-2.9871108,-0.1831503\PG=C01 [X(C6H9O1)]\\@

MP2/6-311G(d,p)

1\1\GINC-GOMBERG14\FTS\UMP2-FC\6-311G(d,p)\C6H9O1(2)\AHANCOCK\22-Apr-2
013\1\\#P Geom=AllCheck Guess=Read MP2/6-311G** freq=noraman opt=(grad
,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C,1,B1\C,2,B2
,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,0\H,3,B6,
2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H
,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0\C,1,B13,
6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\B2=1.5147
6491\B3=1.53586039\B4=1.35382903\B5=1.18473997\B6=1.096059\B7=1.097151
88\B8=1.09639258\B9=1.09390384\B10=1.0892583\B11=1.08374408\B12=1.0856
0997\B13=1.52313862\B14=1.09492109\B15=1.09799793\A1=92.39428236\A2=11
2.26512891\A3=104.73536131\A4=128.70576714\A5=109.28869534\A6=108.5220
9505\A7=109.60229527\A8=110.89213205\A9=91.91957345\A10=121.435269\A11
=120.83697558\A12=130.51390837\A13=108.8923227\A14=107.07098646\D1=25.
25433005\D2=-139.54593786\D3=43.27449645\D4=147.65213246\D5=-95.628490
99\D6=68.94242848\D7=-172.26330943\D8=-76.72405235\D9=-86.74834968\D10
=87.24264132\D11=160.05130257\D12=43.49522226\D13=-73.6205338\B1=2.175
2001\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.2990162\MP2=-308.3316
564\PUHF=-307.3164374\PMP2-0=-308.3465902\S2=0.97954\S2-1=0.912077\S2A
=0.761329\RMSD=6.453e-09\RMSF=2.514e-05\Dipole=0.9240653,0.1523974,0.1
567244\PG=C01 [X(C6H9O1)]\\@

MP2/6-311++G(d,p)

1\1\GINC-GOMBERG14\FTS\UMP2-FC\6-311++G(d,p)\C6H9O1(2)\AHANCOCK\22-Apr
-2013\1\\#P Geom=AllCheck Guess=Read MP2/6-311++G** freq=noraman opt=(
grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C,1,B1\C,
2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,0\H,3
,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7
,0\H,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0\C,1,
B13,6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\B2=1.
51471025\B3=1.53608363\B4=1.35445929\B5=1.18622493\B6=1.09614162\B7=1.
09731766\B8=1.09669624\B9=1.0939498\B10=1.08946004\B11=1.08401188\B12=
1.08604201\B13=1.51993404\B14=1.09518888\B15=1.09832228\A1=92.29039598
\A2=112.30273736\A3=104.82170858\A4=128.63994253\A5=109.21401213\A6=10
8.53850168\A7=109.75559639\A8=110.85946782\A9=91.67648172\A10=121.4377
4075\A11=120.81353528\A12=130.77422716\A13=108.89205997\A14=106.955354

35\D1=25.33716843\D2=-139.60737262\D3=44.01382228\D4=147.64280655\D5=-
95.71856249\D6=69.13271452\D7=-172.12037857\D8=-75.89517145\D9=-86.441
65216\D10=87.24036573\D11=161.09272724\D12=42.75981551\D13=-74.3093435
\B1=2.17868799\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.3037388\MP2
=-308.341938\PUHF=-307.3208938\PMP2-0=-308.3566323\S2=0.976303\S2-1=0.
909509\S2A=0.761012\RMSD=5.392e-09\RMSF=1.373e-05\Dipole=1.0263269,0.1
759243,0.1972026\PG=C01 [X(C6H9O1)]\\@

MP2/cc-pVDZ

1\1\GINC-GOMBERG17\FTS\UMP2-FC\CC-pVDZ\C6H9O1(2)\AHANCOCK\22-Apr-2013\
1\\#P Geom=AllCheck Guess=Read MP2/cc-pVDZ freq=noraman opt=(grad,nofr
eeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C,1,B1\C,2,B2,1,A1
\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,0\H,3,B6,2,A5,
1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,0\H,2,B1
0,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0\C,1,B13,6,A12
,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\B2=1.51802486\
B3=1.53798236\B4=1.36191974\B5=1.19096727\B6=1.10466938\B7=1.1058582\B
8=1.1056607\B9=1.10245465\B10=1.09817285\B11=1.0930569\B12=1.09492658\
B13=1.52837786\B14=1.10341904\B15=1.1067605\A1=92.2854747\A2=112.32820
049\A3=105.436916\A4=129.27816043\A5=109.34716859\A6=108.59092359\A7=1
09.70635018\A8=110.9949979\A9=91.27086298\A10=121.35483144\A11=120.861
00806\A12=130.4941794\A13=109.21398498\A14=106.87667517\D1=25.24439259
\D2=-139.82517721\D3=44.60418399\D4=147.65199044\D5=-95.83420114\D6=68
.83009439\D7=-172.67210073\D8=-75.06510864\D9=-86.49635559\D10=87.4325
2995\D11=161.9829894\D12=41.27909631\D13=-75.64781732\B1=2.18545047\\V
ersion=AM64L-G09RevC.01\State=2-A\HF=-307.2474757\MP2=-308.2242549\PUH
F=-307.2651496\PMP2-0=-308.2394379\S2=0.986018\S2-1=0.917491\S2A=0.761
972\RMSD=8.271e-09\RMSF=2.811e-05\Dipole=0.9037392,0.1458742,0.1424644
\PG=C01 [X(C6H9O1)]\\@

MP2/aug-cc-pVDZ

1\1\GINC-GOMBERG17\FTS\UMP2-FC\Aug-CC-pVDZ\C6H9O1(2)\AHANCOCK\22-Apr-2
013\1\\#P Geom=AllCheck Guess=Read MP2/aug-cc-pVDZ freq=noraman opt=(g
rad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\C,1,B1\C,2
,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,2,B4,1,A3,4,D2,0\O,1,B5,2,A4,5,D3,0\H,3,
B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,4,B8,3,A7,2,D6,0\H,4,B9,3,A8,2,D7,
0\H,2,B10,1,A9,6,D8,0\H,5,B11,2,A10,1,D9,0\H,5,B12,2,A11,1,D10,0\C,1,B
13,6,A12,2,D11,0\H,14,B14,1,A13,6,D12,0\H,14,B15,1,A14,6,D13,0\\B2=1.5
1948231\B3=1.54116539\B4=1.36166571\B5=1.19687904\B6=1.10313344\B7=1.1
0438058\B8=1.10362731\B9=1.10110046\B10=1.09656485\B11=1.09120567\B12=
1.09331905\B13=1.52630389\B14=1.10205302\B15=1.10526417\A1=92.58739781
\A2=112.23506212\A3=103.48083411\A4=128.61968392\A5=109.28137824\A6=10
8.45856724\A7=109.85299973\A8=110.78473167\A9=91.63914617\A10=121.4651
286\A11=120.80156992\A12=130.40497488\A13=108.65939297\A14=107.0005399
\D1=24.71541045\D2=-139.14548563\D3=43.09433988\D4=147.10504046\D5=-96
.21832892\D6=69.49800311\D7=-171.73472813\D8=-76.62386036\D9=-86.69623
532\D10=87.95626965\D11=158.69386177\D12=43.90312916\D13=-73.12509505\
B1=2.17711713\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.2623425\MP2=
-308.282314\PUHF=-307.2795371\PMP2-0=-308.2970733\S2=0.980051\S2-1=0.9
1292\S2A=0.761705\RMSD=9.496e-09\RMSF=5.177e-06\Dipole=1.0357286,0.179
1079,0.2541455\PG=C01 [X(C6H9O1)]\\@

ROMP2/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.351620

QCISD/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.413023

CCSD(T)/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.454847

ROMP2/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.352924

QCISD/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.414135

CCSD(T)/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.456445

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.291424

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.357221

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.397570

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.293658

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.359169

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.400258

Transition State 3 X=CH2 endo Chair

HF/6-31G(d)

1\1\GINC-GOMBERG19\FTS\UHF\6-31G(d)\C6H9O1(2)\CARLHS\06-Jan-2014\1\\#U
HF/6-31G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoint gu
ess=read\\acyl radical endo transition state\\0,2\C\O,1,B1\C,1,B2,2,A1
\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,B6,3,A5,
1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,0\C,8,B1
0,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,1,B13,2,A
12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=1.1722791
8\B3=1.07521497\B4=1.07673656\B5=1.38724171\B6=1.07744088\B7=1.5041421
8\B8=1.0853243\B9=1.08792865\B10=1.5409854\B11=1.08629461\B12=1.086483
86\B13=1.52013085\B14=1.08657782\B15=1.08544595\A1=123.60083106\A2=101
.99776034\A3=92.89535168\A4=95.61896761\A5=119.01075522\A6=119.6820972
4\A7=111.15456179\A8=110.20728273\A9=109.99390388\A10=109.80312338\A11
=109.4205516\A12=127.6563238\A13=107.81554993\A14=107.81091303\D1=-15.
37069107\D2=-132.14695769\D3=107.63692365\D4=-94.25329035\D5=63.992939
07\D6=-195.93764195\D7=45.56453959\D8=-74.90702454\D9=-180.09582603\D1
0=-63.2259521\D11=155.94204757\D12=131.12136987\D13=14.43599535\B2=2.1
9017115\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.2223732\S2=1.02788
9\S2-1=0.\S2A=0.763726\RMSD=8.663e-09\RMSF=1.935e-05\Dipole=-0.2493668
,-0.2580895,-1.0815695\Quadrupole=2.1261747,2.4096197,-4.5357943,0.023
5202,1.5490837,-1.8588919\PG=C01 [X(C6H9O1)]\\@

HF/6-311G(d,p)

1\1\GINC-GOMBERG16\FTS\UHF\6-311G(d,p)\C6H9O1(2)\CARLHS\06-Jan-2014\1\
\#UHF/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoi
nt guess=read\\Acyl radical endo transition state\\0,2\C\O,1,B1\C,1,B2
,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,B6,
3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,0\C
,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,1,B1
3,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=1.16

535564\B3=1.0757299\B4=1.07728486\B5=1.38699315\B6=1.07815164\B7=1.503
79407\B8=1.08544851\B9=1.08842903\B10=1.54046421\B11=1.08663292\B12=1.
08724005\B13=1.51936735\B14=1.08709096\B15=1.08591338\A1=123.3701044\A
2=101.96145732\A3=92.90610144\A4=95.90699235\A5=119.03899582\A6=119.53
479321\A7=111.12084564\A8=110.15420992\A9=109.97663617\A10=109.7749214
7\A11=109.34132524\A12=128.05988206\A13=107.51019585\A14=107.71158173\
D1=-13.62134283\D2=-130.51907015\D3=109.36614434\D4=-94.41342375\D5=63
.80566886\D6=-195.74167926\D7=45.72042952\D8=-74.77234477\D9=-180.0209
7618\D10=-63.19280509\D11=157.56991969\D12=129.32309998\D13=12.70756\B
2=2.18226445\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.2976013\S2=1.
019642\S2-1=0.\S2A=0.763053\RMSD=3.774e-09\RMSF=4.608e-05\Dipole=-0.29
78621,-0.2459137,-1.0542528\Quadrupole=1.9650852,2.4677773,-4.4328625,
0.0039384,1.645478,-1.772898\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/6-311G(d,p)
1\1\GINC-GOMBERG19\FTS\UBHandHLYP\6-311G(d,p)\C6H9O1(2)\CARLHS\06-Jan-
2014\1\\#bhandhlyp/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze)
geom=checkpoint guess=read\\Acyl radical endo transition state\\0,2\C\
O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2
,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,
6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6
,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D
13,0\\B1=1.17491292\B3=1.0761759\B4=1.07779802\B5=1.35811486\B6=1.0787
3115\B7=1.49273898\B8=1.08589659\B9=1.08897531\B10=1.53658416\B11=1.08
798299\B12=1.08739053\B13=1.51782666\B14=1.08705888\B15=1.08684191\A1=
120.66177099\A2=101.08500571\A3=92.84164489\A4=93.04065252\A5=119.2958
6056\A6=120.55078974\A7=111.60851671\A8=110.309651\A9=109.12148158\A10
=110.01495697\A11=109.58017852\A12=127.25741505\A13=108.4512655\A14=10
7.03071321\D1=-27.24231255\D2=-144.26560411\D3=95.16869823\D4=-93.9834
248\D5=68.49196587\D6=-198.53437459\D7=42.24157223\D8=-77.47900549\D9=
-181.98106504\D10=-64.57863401\D11=144.53801399\D12=144.24183847\D13=2
7.31822748\B2=2.15899637\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.0
712867\S2=0.811537\S2-1=0.\S2A=0.750702\RMSD=5.673e-09\RMSF=1.544e-05\
Dipole=-0.2178343,-0.3902836,-0.952626\Quadrupole=1.6046254,1.6692102,
-3.2738357,0.2900876,1.8077322,-1.9651329\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/6-311++G(d,p)
1\1\GINC-GOMBERG19\FTS\UBHandHLYP\6-311++G(d,p)\C6H9O1(2)\CARLHS\07-Ja
n-2014\1\\#bhandhlyp/6-311++G** opt=(grad,ts,readfc,noeigentest,nofree
ze) geom=checkpoint guess=read\\Acyl radical endo transition state\\0,
2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,
A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8
,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A
11,6,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14
,2,D13,0\\B1=1.17630911\B3=1.07619789\B4=1.0777735\B5=1.35865137\B6=1.
0787982\B7=1.49250823\B8=1.08593007\B9=1.08896996\B10=1.53647142\B11=1
.08802835\B12=1.08743837\B13=1.51565262\B14=1.08722013\B15=1.08702583\
A1=120.32911834\A2=101.10906011\A3=92.87692934\A4=92.8106062\A5=119.27
578508\A6=120.59412078\A7=111.58283855\A8=110.29067514\A9=109.10675804
\A10=109.96361767\A11=109.64324391\A12=127.46486621\A13=108.37536087\A
14=107.16504808\D1=-27.06621078\D2=-144.1304366\D3=95.30361752\D4=-93.
9728365\D5=68.63877166\D6=-198.69713582\D7=42.08170835\D8=-77.65467687
\D9=-182.25441108\D10=-64.87228293\D11=144.73611137\D12=144.2595695\D1
3=27.38696611\B2=2.1573487\\Version=AM64L-G09RevC.01\State=2-A\HF=-309
.0765699\S2=0.809825\S2-1=0.\S2A=0.750679\RMSD=8.631e-09\RMSF=1.743e-0

5\Dipole=-0.2270648,-0.423421,-1.0456616\Quadrupole=1.760483,1.8380926
,-3.5985756,0.3554224,2.0249862,-2.0937944\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-GOMBERG19\FTS\UBHandHLYP\CC-pVDZ\C6H9O1(2)\CARLHS\06-Jan-2014
\1\\#bhandhlyp/cc-pVDZ opt=(grad,ts,readfc,noeigentest,nofreeze) geom=
checkpoint guess=read\\Acyl radical endo transition state\\0,2\C\O,1,B
1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0
\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,
3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,
0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\
\B1=1.18002521\B3=1.08437875\B4=1.08583374\B5=1.36160541\B6=1.08715521
\B7=1.49414746\B8=1.09369918\B9=1.09692278\B10=1.53557577\B11=1.095982
71\B12=1.09567716\B13=1.51901015\B14=1.09513826\B15=1.0946643\A1=120.9
0833871\A2=101.08885663\A3=92.22697805\A4=93.06623821\A5=119.2195918\A
6=120.5516771\A7=111.67477173\A8=110.24461192\A9=109.19311753\A10=110.
0493991\A11=109.58772864\A12=127.17561962\A13=108.35584197\A14=106.947
0086\D1=-26.81824005\D2=-143.89171356\D3=95.63562915\D4=-94.03268787\D
5=68.19281192\D6=-198.76245627\D7=42.08931098\D8=-77.58045941\D9=-181.
59029866\D10=-64.31234126\D11=144.51058826\D12=143.68870526\D13=26.929
33542\B2=2.17298348\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.009284
6\S2=0.812276\S2-1=0.\S2A=0.750713\RMSD=8.714e-09\RMSF=2.232e-05\Dipol
e=-0.2119501,-0.3770523,-0.9135377\Quadrupole=1.5770904,1.5596124,-3.1
367028,0.2680148,1.6822946,-1.8763943\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\Aug-CC-pVDZ\C6H9O1(2)\CARLHS\07-Jan-
2014\1\\#bhandhlyp/aug-cc-pVDZ opt=(grad,ts,readfc,noeigentest,nofreez
e) geom=checkpoint guess=read\\Acyl radical endo transition state\\0,2
\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A
4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,
B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A1
1,6,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,
2,D13,0\\B1=1.18250997\B3=1.08163456\B4=1.08308126\B5=1.36189832\B6=1.
08444089\B7=1.493622\B8=1.09094387\B9=1.09376811\B10=1.53639928\B11=1.
09297457\B12=1.09230628\B13=1.51664074\B14=1.09204424\B15=1.09181702\A
1=119.86270475\A2=101.01815373\A3=92.97973655\A4=92.0658578\A5=119.149
79591\A6=120.81054479\A7=111.54180869\A8=110.29691732\A9=108.98072781\
A10=109.9563803\A11=109.69129284\A12=127.16769891\A13=108.55447815\A14
=106.97560496\D1=-28.82531081\D2=-146.11036654\D3=93.30438932\D4=-93.6
5983015\D5=69.23210573\D6=-199.00902982\D7=41.54532537\D8=-78.10409101
\D9=-182.45387381\D10=-64.87817534\D11=143.09030717\D12=146.59819343\D
13=29.46369854\B2=2.15869824\\Version=AM64L-G09RevC.01\State=2-A\HF=-3
09.0293378\S2=0.808628\S2-1=0.\S2A=0.750695\RMSD=5.173e-09\RMSF=1.086e
-05\Dipole=-0.1862686,-0.4413282,-1.0364674\Quadrupole=1.7158429,1.707
6584,-3.4235013,0.3889657,2.0306169,-2.1385853\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\CC-pVTZ\C6H9O1(2)\CARLHS\07-Jan-2014
\1\\#bhandhlyp/cc-pVTZ opt=(grad,ts,readfc,noeigentest,nofreeze) geom=
checkpoint guess=read\\Acyl radical endo transition state\\0,2\C\O,1,B
1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0
\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,
3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,
0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\

\B1=1.17480551\B3=1.07368704\B4=1.07522959\B5=1.35481083\B6=1.07628761
\B7=1.4890736\B8=1.08353083\B9=1.08653759\B10=1.5331416\B11=1.08556605
\B12=1.08498169\B13=1.51295471\B14=1.08469051\B15=1.08451224\A1=120.29
496148\A2=101.07819657\A3=92.98223973\A4=92.75851168\A5=119.26341684\A
6=120.64959723\A7=111.64745348\A8=110.28008931\A9=109.1105184\A10=110.
00549245\A11=109.60567497\A12=127.34503386\A13=108.51429855\A14=107.06
341924\D1=-27.43638804\D2=-144.50403358\D3=94.91450687\D4=-93.82981231
\D5=68.71716026\D6=-198.72870452\D7=42.01779424\D8=-77.63928475\D9=-18
2.2330362\D10=-64.81629662\D11=144.45499119\D12=144.60953051\D13=27.66
796363\B2=2.14946959\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.10280
57\S2=0.809563\S2-1=0.\S2A=0.750706\RMSD=4.172e-09\RMSF=1.267e-05\Dipo
le=-0.2087092,-0.4019895,-0.9787641\Quadrupole=1.629126,1.6637944,-3.2
929205,0.3155482,1.8450559,-2.0037259\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/aug-cc-pVTZ

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\Aug-CC-pVTZ\C6H9O1(2)\CARLHS\07-Jan-
2014\1\\#bhandhlyp/aug-cc-pVTZ opt=(grad,ts,readfc,noeigentest,nofreez
e) geom=checkpoint guess=read\\Acyl radical endo transition state\\0,2
\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A
4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,
B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A1
1,6,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,
2,D13,0\\B1=1.17489234\B3=1.07360596\B4=1.07513075\B5=1.35480087\B6=1.
07624577\B7=1.48889732\B8=1.0834067\B9=1.08639037\B10=1.53305646\B11=1
.08545208\B12=1.0848501\B13=1.5123613\B14=1.08455062\B15=1.08445928\A1
=120.13809222\A2=101.08474013\A3=93.02154502\A4=92.63746083\A5=119.262
78213\A6=120.66911048\A7=111.6342506\A8=110.27095471\A9=109.09622159\A
10=109.98628467\A11=109.62462779\A12=127.50042236\A13=108.45899961\A14
=107.11789024\D1=-27.43406971\D2=-144.5306917\D3=94.89812\D4=-93.79916
545\D5=68.85233184\D6=-198.77995448\D7=41.94866211\D8=-77.71471075\D9=
-182.40536331\D10=-64.97666503\D11=144.50941882\D12=144.75289241\D13=2
7.81240416\B2=2.14876726\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.1
063669\S2=0.808451\S2-1=0.\S2A=0.750692\RMSD=4.857e-09\RMSF=1.771e-05\
Dipole=-0.2081441,-0.4152141,-1.0252306\Quadrupole=1.6974071,1.7617672
,-3.4591743,0.3458704,1.9784506,-2.0517371\PG=C01 [X(C6H9O1)]\\@

MP2/6-311G(d,p)

1\1\GINC-GOMBERG01\FTS\UMP2-FC\6-311G(d,p)\C6H9O1(2)\CARLHS\07-Jan-201
4\1\\#mp2=direct/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) ge
om=checkpoint guess=read\\Acyl radical endo transition state\\0,2\C\O,
1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D
3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,
A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D
10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13
,0\\B1=1.19759942\B3=1.08523881\B4=1.08677425\B5=1.3482869\B6=1.087936
69\B7=1.49594597\B8=1.09479328\B9=1.09713508\B10=1.5451072\B11=1.09752
55\B12=1.09640501\B13=1.53172273\B14=1.09548508\B15=1.09567673\A1=120.
07787307\A2=99.89096967\A3=94.4378899\A4=90.53167201\A5=119.2324876\A6
=121.19896742\A7=111.87588733\A8=110.37174447\A9=107.73706829\A10=110.
31673903\A11=109.74009719\A12=126.0642158\A13=108.8928161\A14=106.6865
8202\D1=-34.36132153\D2=-152.06564966\D3=87.32497128\D4=-91.42064312\D
5=72.9649173\D6=-201.187836\D7=38.40990321\D8=-80.14169167\D9=-183.017
10978\D10=-64.42644639\D11=139.63596597\D12=153.43003952\D13=35.919612
69\B2=2.10270429\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.2916796\M
P2=-308.3310876\PUHF=-307.3076062\PMP2-0=-308.3447573\S2=0.963\S2-1=0.

90103\S2A=0.759551\RMSD=3.863e-09\RMSF=2.322e-05\Dipole=-0.1273238,-0.
4381404,-0.8209793\PG=C01 [X(C6H9O1)]\\@

MP2/6-311++G(d,p)

1\1\GINC-GOMBERG19\FTS\UMP2-FC\6-311++G(d,p)\C6H9O1(2)\CARLHS\07-Jan-2
014\1\\#mp2=direct/6-311++G** opt=(grad,ts,readfc,noeigentest,nofreeze
) geom=checkpoint guess=read\\Acyl radical endo transition state\\0,2\
C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4
,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B
9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11
,6,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2
,D13,0\\B1=1.20046589\B3=1.08527092\B4=1.08687121\B5=1.34897368\B6=1.0
8819136\B7=1.49570345\B8=1.09479378\B9=1.09712225\B10=1.5453016\B11=1.
09754574\B12=1.09659256\B13=1.52884514\B14=1.09581379\B15=1.09590378\A
1=119.60652885\A2=99.95773846\A3=94.51584543\A4=90.00255389\A5=119.213
19499\A6=121.29863652\A7=111.81172292\A8=110.40886751\A9=107.62086686\
A10=110.28487193\A11=109.82619146\A12=126.32156815\A13=108.89558514\A1
4=106.70042718\D1=-34.3179616\D2=-152.06641245\D3=87.35488781\D4=-91.3
9598733\D5=73.38307343\D6=-201.63472644\D7=37.92870434\D8=-80.66764273
\D9=-183.27659509\D10=-64.72800335\D11=139.83314618\D12=153.64925454\D
13=36.26371391\B2=2.09982197\\Version=AM64L-G09RevC.01\State=2-A\HF=-3
07.29608\MP2=-308.341539\PUHF=-307.3116524\PMP2-0=-308.3548879\S2=0.95
8153\S2-1=0.897163\S2A=0.759135\RMSD=5.797e-09\RMSF=2.215e-05\Dipole=-
0.1291957,-0.4939299,-0.9348908\PG=C01 [X(C6H9O1)]\\@

MP2/cc-pVDZ

1\1\GINC-GOMBERG02\FTS\UMP2-FC\CC-pVDZ\C6H9O1(2)\CARLHS\07-Jan-2014\1\
\#mp2=direct/cc-pVDZ opt=(grad,ts,readfc,noeigentest,nofreeze) geom=ch
eckpoint guess=read\\Acyl radical endo transition state\\0,2\C\O,1,B1\
C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H
,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,
D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\
C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B
1=1.2031984\B3=1.09405686\B4=1.0954515\B5=1.35581054\B6=1.09699544\B7=
1.50058076\B8=1.10323496\B9=1.105941\B10=1.54671648\B11=1.1063736\B12=
1.10557921\B13=1.53688783\B14=1.10466437\B15=1.10449275\A1=120.6567585
\A2=99.9502679\A3=93.40481794\A4=91.31086309\A5=119.23247701\A6=120.92
087202\A7=111.99686247\A8=110.33619989\A9=107.9398186\A10=110.35410892
\A11=109.73265783\A12=126.21268311\A13=108.82282003\A14=106.71223985\D
1=-32.55052158\D2=-150.08730698\D3=89.38778742\D4=-91.94928294\D5=72.0
0602232\D6=-200.80326968\D7=39.04938733\D8=-79.62685637\D9=-182.360820
67\D10=-64.1477698\D11=140.96815188\D12=150.59199031\D13=33.44373128\B
2=2.11908338\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.240425\MP2=-3
08.223019\PUHF=-307.2566735\PMP2-0=-308.2369999\S2=0.970657\S2-1=0.907
374\S2A=0.760239\RMSD=8.635e-09\RMSF=2.304e-05\Dipole=-0.1484005,-0.40
78947,-0.7873708\PG=C01 [X(C6H9O1)]\\@

MP2/aug-cc-pVDZ

1\1\GINC-GOMBERG01\FTS\UMP2-FC\Aug-CC-pVDZ\C6H9O1(2)\CARLHS\07-Jan-201
4\1\\#mp2=direct/aug-cc-pVDZ opt=(grad,ts,readfc,noeigentest,nofreeze)
 geom=checkpoint guess=read\\Acyl radical endo transition state\\0,2\C
\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,
2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9
,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,
6,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,

D13,0\\B1=1.21257667\B3=1.09223823\B4=1.09402584\B5=1.35617061\B6=1.09
536391\B7=1.50015112\B8=1.10174263\B9=1.10419318\B10=1.55031395\B11=1.
10472425\B12=1.1037358\B13=1.53378152\B14=1.10307975\B15=1.10299486\A1
=118.92050509\A2=99.56294932\A3=94.79655046\A4=89.16775924\A5=119.0423
2532\A6=121.47187898\A7=111.90072937\A8=110.43685454\A9=107.2833275\A1
0=110.34706521\A11=109.8990671\A12=125.99433719\A13=109.08532435\A14=1
06.57653143\D1=-35.62013182\D2=-153.59845409\D3=85.86033523\D4=-90.669
85594\D5=74.15171699\D6=-202.3215107\D7=37.01688673\D8=-81.47746413\D9
=-183.10986928\D10=-64.41405322\D11=138.783887\D12=155.31960473\D13=37
.8581118\B2=2.09715626\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.255
0312\MP2=-308.2830183\PUHF=-307.2705068\PMP2-0=-308.2962883\S2=0.95792
1\S2-1=0.897067\S2A=0.759383\RMSD=7.347e-09\RMSF=2.603e-05\Dipole=-0.0
802162,-0.5188957,-0.9580816\PG=C01 [X(C6H9O1)]\\@

ROMP2/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.3517556

QCISD/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.4111504

CCSD(T)/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.4538074

ROMP2/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.3531471

QCISD/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.411489

CCSD(T)/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.4548814

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.2924792

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.3560101

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.3972622

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.2947809

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.3572351

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.3994669

Transition State 2 X=O exo Chair

HF/6-31G(d)

1\1\GINC-GOMBERG13\FTS\UHF\6-31G(d)\C5H7O2(2)\AHANCOCK\27-Jan-2012\0\\
#HF/6-31G* opt=(ts,readfc,noeigentest,nofreeze,maxcycles=10000) freq=n
oraman guess=read geom=checkpoint\\Calc E for butenyloxyacyl radical c
yclization\\0,2\C,0.0202080575,0.0304776234,-0.0043360349\C,0.00103390
14,-0.0050998281,2.2125590843\C,1.5107001424,0.005383301,2.1687817225\
C,1.988133666,0.7679025724,0.9395483986\O,1.2942042202,0.30690606,-0.2
117982356\C,-0.7266090389,-1.1128778815,2.6085058519\O,-0.774348058,-0
.2875222035,-0.7978854684\H,1.923527632,0.4738366858,3.0583377599\H,1.
8833193025,-1.0131757249,2.1321078797\H,1.8115381469,1.8322557348,1.04
44253035\H,3.0367220087,0.6100308437,0.7400244599\H,-0.4735894269,0.95
93826513,2.3022608866\H,-1.787009579,-1.0512845916,2.7666327832\H,-0.2
758691449,-2.0880406413,2.6603485858\\Version=AM64L-G09RevB.01\State=2
-A\HF=-343.0577506\S2=1.018688\S2-1=0.\S2A=0.762363\RMSD=7.202e-09\RMS

F=3.860e-05\Dipole=0.9424725,0.4099656,1.4305035\Quadrupole=1.4919745,
3.0218768,-4.5138513,0.1078863,-1.9989134,-0.5498153\PG=C01 [X(C5H7O2)
]\\@

HF/6-311G(d,p)

1\1\GINC-GOMBERG19\FTS\UHF\6-311++G(d,p)\C5H7O2(2)\AHANCOCK\16-Feb-201
2\0\\#HF/6-311++G** opt=(ts,readfc,noeigentest,nofreeze,maxcycles=1000
0) freq=noraman guess=read geom=checkpoint\\Calc E for butenyloxyacyl
radical cyclization\\0,2\C,0.0225036465,0.0271795895,-0.0008424903\C,0
.0024197131,-0.0074043292,2.207081705\C,1.5115608431,0.004756435,2.168
3993268\C,1.9885906774,0.766546339,0.9407014749\O,1.2891272655,0.30946
04095,-0.2103505894\C,-0.7253339151,-1.1136400993,2.6064793316\O,-0.77
87239994,-0.2792008614,-0.7836327412\H,1.9204444452,0.4783030073,3.057
3612237\H,1.8862358809,-1.0137789456,2.1365063998\H,1.8131611031,1.832
053666,1.0459355353\H,3.0367194811,0.605964863,0.7381924569\H,-0.47520
51629,0.9568458292,2.2916625433\H,-1.7872158126,-1.0506253632,2.758186
9637\H,-0.2723223358,-2.088285938,2.6638318367\\Version=AM64L-G09RevB.
01\State=2-A\HF=-343.1500397\S2=1.006545\S2-1=0.\S2A=0.761364\RMSD=6.5
32e-09\RMSF=6.598e-06\Dipole=0.9946645,0.4222161,1.4477537\Quadrupole=
1.6265462,3.2439479,-4.870494,0.0902446,-1.9986308,-0.5261181\PG=C01 [
X(C5H7O2)]\\@

BHandHLYP/6-311G(d,p)

1\1\GINC-GOMBERG10\FTS\UBHandHLYP\6-311G(d,p)\C5H7O2(2)\AHANCOCK\16-Fe
b-2012\0\\#BHandHLYP/6-311G** opt=(ts,readfc,noeigentest,nofreeze,maxc
ycles=10000) freq=noraman guess=read geom=checkpoint\\Calc E for buten
yloxyacyl radical cyclization\\0,2\C,0.0072390781,0.0532058462,0.00216
13223\C,0.0032251477,-0.0087256491,2.2227105943\C,1.5052268935,0.00768
22298,2.1733243722\C,1.9855579953,0.7554944869,0.9449744698\O,1.294969
4638,0.2790519346,-0.2104649425\C,-0.7090172101,-1.1046780878,2.587925
0307\O,-0.7925505994,-0.2746783683,-0.7843417002\H,1.9136754176,0.4885
749887,3.0594867789\H,1.8790574505,-1.0120745952,2.1512941366\H,1.8059
351306,1.8229295991,1.0366148793\H,3.0361203207,0.594775576,0.74841966
52\H,-0.4781152657,0.9553077765,2.2966543836\H,-1.7706747418,-1.051711
1117,2.7490141253\H,-0.2486872508,-2.0769800242,2.6417398612\\Version=
AM64L-G09RevB.01\State=2-A\HF=-344.9867856\S2=0.821881\S2-1=0.\S2A=0.7
50788\RMSD=8.273e-09\RMSF=2.951e-05\Dipole=0.9360452,0.4093908,1.20874
48\Quadrupole=1.4932713,2.750094,-4.2433653,0.1705589,-1.6235692,-0.39
71578\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG13\FTS\UBHandHLYP\6-311++G(d,p)\C5H7O2(2)\AHANCOCK\27-
Jan-2012\0\\#BHandHLYP/6-311++G** opt=(ts,readfc,noeigentest,nofreeze,
maxcycles=10000) freq=noraman guess=read geom=checkpoint\\Calc E for b
utenyloxyacyl radical cyclization\\0,2\C,0.0080439281,0.0517663219,0.0
00226143\C,0.0037734819,-0.0097453815,2.2230148827\C,1.5055421453,0.00
68361964,2.1733458444\C,1.9861532362,0.7555285483,0.9461931422\O,1.292
7196938,0.2819650212,-0.2106551715\C,-0.7088765601,-1.1057614046,2.589
5646648\O,-0.7947978295,-0.2696489099,-0.7871046946\H,1.9131406452,0.4
896464489,3.0588847736\H,1.8809780986,-1.0124488389,2.1539258733\H,1.8
074457221,1.8230431897,1.0370401014\H,3.036225452,0.5934099004,0.74767
01153\H,-0.4792372188,0.953917517,2.2920012262\H,-1.7709172644,-1.0525
399634,2.7485928171\H,-0.2482317004,-2.0777940438,2.6468132592\\Versio
n=AM64L-G09RevB.01\State=2-A\HF=-344.9941181\S2=0.819702\S2-1=0.\S2A=0

.750747\RMSD=8.916e-09\RMSF=1.408e-05\Dipole=0.9799846,0.424964,1.3073
412\Quadrupole=1.6354853,3.004754,-4.6402393,0.1896272,-1.716563,-0.44
623\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-GOMBERG14\FTS\UBHandHLYP\CC-pVDZ\C5H7O2(2)\AHANCOCK\21-Apr-20
13\0\\#BHandHLYP/cc-pVDZ opt=(ts,readfc,noeigentest,nofreeze,maxcycles
=10000) freq=noraman guess=read geom=checkpoint\\Calc E for butenyloxy
acyl radical cyclization\\0,2\C,0.0083456587,0.0530593322,-0.005326139
5\C,0.0024490356,-0.0108604176,2.2263844568\C,1.5045678249,0.004867316
3,2.169386337\C,1.9832836044,0.7563913933,0.9426442914\O,1.3008580977,
0.2822367295,-0.2163690372\C,-0.7129635112,-1.1075706003,2.5989455035\
O,-0.787142821,-0.2703279145,-0.8051897994\H,1.9210813104,0.4863311993
,3.0612034971\H,1.8808338859,-1.0224064657,2.1443932998\H,1.8013221801
,1.8318298467,1.0392728586\H,3.0439728753,0.6012379373,0.7499245248\H,
-0.4832136942,0.960766726,2.2935360114\H,-1.7823249119,-1.0500451719,2
.7638561944\H,-0.2491077046,-2.0873353091,2.6568509782\\Version=AM64L-
G09RevC.01\State=2-A\HF=-344.9179627\S2=0.823377\S2-1=0.\S2A=0.750814\
RMSD=6.645e-09\RMSF=3.418e-05\Dipole=0.9014363,0.3950137,1.1617193\Qua
drupole=1.4245297,2.5672196,-3.9917493,0.162025,-1.5585683,-0.3534093\
PG=C01 [X(C5H7O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\Aug-CC-pVDZ\C5H7O2(2)\AHANCOCK\27-Ja
n-2012\0\\#BHandHLYP/aug-cc-pVDZ opt=(ts,readfc,noeigentest,nofreeze,m
axcycles=10000) freq=noraman guess=read geom=checkpoint\\Calc E for bu
tenyloxyacyl radical cyclization\\0,2\C,0.0040333174,0.057085159,-0.00
39259517\C,0.0040001992,-0.0089491964,2.2299118981\C,1.5063881176,0.00
75429553,2.1743974962\C,1.9868369719,0.7553098046,0.9456486781\O,1.294
5237992,0.2808666729,-0.2149255723\C,-0.7107247526,-1.1090664803,2.591
6949313\O,-0.7965974907,-0.2694149791,-0.8003448625\H,1.9179344932,0.4
955372605,3.0616311871\H,1.8829034145,-1.0163706577,2.1550619841\H,1.8
083313806,1.8282070627,1.0361660153\H,3.0420220926,0.5897740655,0.7467
946777\H,-0.4829809831,0.9591072643,2.2950022164\H,-1.7784263755,-1.05
59644612,2.7516922179\H,-0.2462823542,-2.0854898683,2.6507080612\\Vers
ion=AM64L-G09RevB.01\State=2-A\HF=-344.941848\S2=0.819669\S2-1=0.\S2A=
0.750769\RMSD=6.197e-09\RMSF=4.970e-06\Dipole=0.9753883,0.4182318,1.27
68306\Quadrupole=1.5833333,2.9257766,-4.5091099,0.1594385,-1.8001393,-
0.4401177\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-GOMBERG14\FTS\UBHandHLYP\CC-pVTZ\C5H7O2(2)\AHANCOCK\21-Apr-20
13\0\\#BHandHLYP/cc-pVTZ opt=(ts,readfc,noeigentest,nofreeze,maxcycles
=10000) freq=noraman guess=read geom=checkpoint\\Calc E for butenyloxy
acyl radical cyclization\\0,2\C,0.0079894189,0.0516579492,0.0023781324
\C,0.003750517,-0.0111854109,2.220877921\C,1.5021498424,0.0064344728,2
.1703345384\C,1.9834634944,0.7547635052,0.9468610497\O,1.2907125337,0.
2881854681,-0.2091782534\C,-0.7057418598,-1.103102423,2.589646471\O,-0
.7908772544,-0.272666677,-0.7862143416\H,1.9098551353,0.4862666193,3.0
546353986\H,1.8765143765,-1.0106549406,2.1494246697\H,1.8106542959,1.8
207965167,1.0426968552\H,3.0317978196,0.5904523049,0.751550936\H,-0.47
7985782,0.9504286114,2.2867573159\H,-1.7651417979,-1.0509171388,2.7500
177294\H,-0.2451789097,-2.0722842556,2.6497245546\\Version=AM64L-G09Re
vC.01\State=2-A\HF=-345.0239902\S2=0.819291\S2-1=0.\S2A=0.750761\RMSD=
2.354e-09\RMSF=4.276e-06\Dipole=0.9596018,0.4115971,1.2021664\Quadrupo

le=1.4794937,2.732806,-4.2122997,0.1340958,-1.6992981,-0.3851364\PG=C0
1 [X(C5H7O2)]\\@

BHandHLYP/aug-cc-pVTZ

1\1\GINC-GOMBERG01\FTS\UBHandHLYP\Aug-CC-pVDZ\C5H7O2(2)\AHANCOCK\27-Ja
n-2012\0\\#BHandHLYP/aug-cc-pVDZ opt=(ts,readfc,noeigentest,nofreeze,m
axcycles=10000) freq=noraman guess=read geom=checkpoint\\Calc E for bu
tenyloxyacyl radical cyclization\\0,2\C,0.0040333174,0.057085159,-0.00
39259517\C,0.0040001992,-0.0089491964,2.2299118981\C,1.5063881176,0.00
75429553,2.1743974962\C,1.9868369719,0.7553098046,0.9456486781\O,1.294
5237992,0.2808666729,-0.2149255723\C,-0.7107247526,-1.1090664803,2.591
6949313\O,-0.7965974907,-0.2694149791,-0.8003448625\H,1.9179344932,0.4
955372605,3.0616311871\H,1.8829034145,-1.0163706577,2.1550619841\H,1.8
083313806,1.8282070627,1.0361660153\H,3.0420220926,0.5897740655,0.7467
946777\H,-0.4829809831,0.9591072643,2.2950022164\H,-1.7784263755,-1.05
59644612,2.7516922179\H,-0.2462823542,-2.0854898683,2.6507080612\\Vers
ion=AM64L-G09RevB.01\State=2-A\HF=-344.941848\S2=0.819669\S2-1=0.\S2A=
0.750769\RMSD=6.197e-09\RMSF=4.970e-06\Dipole=0.9753883,0.4182318,1.27
68306\Quadrupole=1.5833333,2.9257766,-4.5091099,0.1594385,-1.8001393,-
0.4401177\PG=C01 [X(C5H7O2)]\\@

MP2/6-311G(d,p)

1\1\GINC-GOMBERG11\FTS\UMP2-FC\6-311G(d,p)\C5H7O2(2)\AHANCOCK\21-Apr-2
013\0\\#MP2/6-311G** opt=(ts,readfc,noeigentest,nofreeze,maxcycles=100
00) freq=noraman guess=read geom=checkpoint\\Calc E for butenyloxyacyl
 radical cyclization\\0,2\C,-0.002867768,0.0628789857,0.034459013\C,0.
006613884,0.0050870323,2.2342094629\C,1.5141202172,0.0120075819,2.1872
020726\C,1.9895126441,0.7498985332,0.9431869997\O,1.3167648288,0.21123
01641,-0.2104169407\C,-0.7046812443,-1.0969306134,2.5569004204\O,-0.83
28374827,-0.279798644,-0.7405022785\H,1.9267399262,0.5003704912,3.0778
677215\H,1.8804822474,-1.0193040631,2.1602709112\H,1.7708428107,1.8207
015216,1.0129537071\H,3.0539407965,0.6101005141,0.755013843\H,-0.47492
12136,0.9784363323,2.3162944203\H,-1.7769880971,-1.0518841513,2.704539
7763\H,-0.2347597191,-2.0746190829,2.5875338481\\Version=AM64L-G09RevC
.01\State=2-A\HF=-343.1395903\MP2=-344.2131753\PUHF=-343.1574427\PMP2-
0=-344.2284848\S2=0.983471\S2-1=0.915074\S2A=0.761179\RMSD=7.735e-09\R
MSF=1.476e-05\Dipole=0.8429895,0.3765245,1.0628857\PG=C01 [X(C5H7O2)]\
\@

MP2/6-311++G(d,p)

1\1\GINC-GOMBERG10\FTS\UMP2-FC\6-311++G(d,p)\C5H7O2(2)\AHANCOCK\30-Jan
-2012\0\\#MP2/6-311++G** opt=(ts,readfc,noeigentest,nofreeze,maxcycles
=10000) freq=noraman guess=read geom=checkpoint\\Calc E for butenyloxy
acyl radical cyclization\\0,2\C,-0.0026839927,0.0592341589,0.029580722
7\C,0.0063044166,0.003576226,2.2347347373\C,1.5137440993,0.0095778386,
2.1855554843\C,1.9909395313,0.7527733522,0.9460470541\O,1.3137387946,0
.2210722255,-0.2125819439\C,-0.7050874074,-1.0973801139,2.562962051\O,
-0.8333835159,-0.2795714288,-0.7487367371\H,1.9267630189,0.4973789531,
3.0765383514\H,1.8819014076,-1.0213755823,2.159019055\H,1.7754082074,1
.8240238058,1.0165316032\H,3.0544213507,0.6089575501,0.7548823099\H,-0
.4768421262,0.9769471633,2.310149174\H,-1.7780445646,-1.0516840456,2.7
074046058\H,-0.2352173895,-2.0753555013,2.5974265091\\Version=AM64L-G0
9RevB.01\State=2-A\HF=-343.1457871\MP2=-344.2275069\PUHF=-343.1633505\
PMP2-0=-344.2425584\S2=0.980204\S2-1=0.912523\S2A=0.76082\RMSD=8.877e-
09\RMSF=9.202e-06\Dipole=0.8951236,0.4014892,1.1821647\PG=C01 [X(C5H7O

2)]\\@

MP2/cc-pVDZ

1\1\GINC-GOMBERG17\FTS\UMP2-FC\CC-pVDZ\C5H7O2(2)\AHANCOCK\21-Apr-2013\
0\\#MP2/cc-pVDZ opt=(ts,readfc,noeigentest,nofreeze,maxcycles=10000) f
req=noraman guess=read geom=checkpoint\\Calc E for butenyloxyacyl radi
cal cyclization\\0,2\C,-0.0028372949,0.0578566318,0.0240784653\C,0.004
6627734,0.0002511573,2.2336214194\C,1.5153106556,0.0073044846,2.182459
6133\C,1.9912060677,0.7545112563,0.9406553658\O,1.3216957706,0.2272666
229,-0.222777693\C,-0.7127296962,-1.1025318256,2.57289631\O,-0.8309925
647,-0.2768513342,-0.7657342552\H,1.9340813346,0.4958784534,3.08078190
89\H,1.886990079,-1.0315002373,2.1542554312\H,1.7763632488,1.835293147
9,1.0213808376\H,3.0657859357,0.6192666299,0.7542758376\H,-0.482930177
9,0.9816746514,2.3031860374\H,-1.7934925734,-1.0509516522,2.7252759552
\H,-0.2411517284,-2.0892933846,2.6151577434\\Version=AM64L-G09RevC.01\
State=2-A\HF=-343.0794128\MP2=-344.0928007\PUHF=-343.0974788\PMP2-0=-3
44.1083269\S2=0.989531\S2-1=0.920212\S2A=0.761838\RMSD=4.417e-09\RMSF=
2.213e-05\Dipole=0.8200807,0.3633603,1.0332102\PG=C01 [X(C5H7O2)]\\@

MP2/aug-cc-pVDZ

1\1\GINC-GOMBERG10\FTS\UMP2-FC\Aug-CC-pVDZ\C5H7O2(2)\AHANCOCK\30-Jan-2
012\0\\#MP2/aug-cc-pVDZ opt=(ts,readfc,noeigentest,nofreeze,maxcycles=
10000) freq=noraman guess=read geom=checkpoint\\Calc E for butenyloxya
cyl radical cyclization\\0,2\C,-0.0232714516,0.0745726247,0.0393225608
\C,0.0074383449,0.0089782612,2.2465636181\C,1.5198125334,0.020653779,2
.1995506759\C,2.0002371583,0.7456019167,0.9440954292\O,1.3080773651,0.
2016821862,-0.2153339576\C,-0.7052874641,-1.1080055354,2.5438846458\O,
-0.8635040773,-0.2697993927,-0.7428805991\H,1.9300441499,0.5326581592,
3.0871198634\H,1.8941087296,-1.0156964364,2.1961938759\H,1.7957202357,
1.8272819066,0.9983094541\H,3.0674923345,0.5855115514,0.7452813084\H,-
0.4877868588,0.9841303238,2.3220542059\H,-1.7867316813,-1.0705175937,2
.6817077918\H,-0.2243874883,-2.088877149,2.5736441044\\Version=AM64L-G
09RevB.01\State=2-A\HF=-343.0988733\MP2=-344.1633818\PUHF=-343.1163963
\PMP2-0=-344.1784242\S2=0.982461\S2-1=0.914746\S2A=0.761323\RMSD=7.405
e-09\RMSF=1.016e-05\Dipole=0.9099028,0.3949466,1.1951587\PG=C01 [X(C5H
7O2)]\\@

ROMP2/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.235917

QCISD/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.285457

CCSD(T)/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.328010

ROMP2/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.237769

QCISD/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.286747

CCSD(T)/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.329964

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.170896

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.225261

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.266071

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.172828

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.226567

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.267862

Transition State 3 X=O endo Boat

HF/6-31G(d)

1\1\GINC-GOMBERG12\FTS\UHF\6-31G(d)\C5H7O2(2)\AHANCOCK\28-Mar-2013\1\\
#P HF/6-31G* OPT=(grad,readfc,nofreeze,ts,noeigentest) geom=Allcheck g
uess=read freq=noraman\\Benchmark\\0,2\C\O,1,B1\O,1,B2,2,A1\C,1,B3,3,A
2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\C,4,B6,1,A5,3,D4,0\H,7,
B7,4,A6,1,D5,0\C,7,B8,4,A7,1,D6,0\H,9,B9,7,A8,4,D7,0\H,9,B10,7,A9,4,D8
,0\C,2,B11,1,A10,3,D9,0\H,12,B12,2,A11,1,D10,0\H,12,B13,2,A12,1,D11,0\
\B1=1.32550989\B2=1.16923775\B4=1.07496892\B5=1.07531522\B6=1.38624773
\B7=1.07539376\B8=1.50897144\B9=1.08443344\B10=1.08860068\B11=1.422423
13\B12=1.07920251\B13=1.08228675\A1=125.82069877\A2=124.34220666\A3=10
3.44502633\A4=91.75886887\A5=94.06229168\A6=118.94353345\A7=120.306963
3\A8=109.39262373\A9=112.3925755\A10=118.00168659\A11=105.02625654\A12
=109.13499154\D1=-155.86258254\D2=-0.13696404\D3=-116.41174408\D4=122.
36998111\D5=-99.31949911\D6=61.46110032\D7=-149.98002121\D8=91.5105671
5\D9=-183.36690552\D10=-168.62117227\D11=-53.13190081\B3=2.20997918\\V
ersion=AM64L-G09RevC.01\State=2-A\HF=-343.0482291\S2=1.037107\S2-1=0.\
S2A=0.763803\RMSD=8.287e-09\RMSF=4.023e-05\Dipole=-1.5466706,-0.139224
3,0.7965173\Quadrupole=-4.5342394,2.741807,1.7924324,-1.9727082,1.8505
983,0.9047179\PG=C01 [X(C5H7O2)]\\@

HF/6-311G(d,p)

1\1\GINC-GOMBERG12\FTS\UHF\6-311G(d,p)\C5H7O2(2)\AHANCOCK\28-Mar-2013\
 1\\#P Geom=Allcheck Guess=Read HF/6-311G(d,p) Freq=noraman opt=(grad,n
 ofreeze,ts,noeigentest,readfc)\\Benchmark\\0,2\C\O,1,B1\O,1,B2,2,A1\C,
 1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\C,4,B6,1,A5,3,D
 4,0\H,7,B7,4,A6,1,D5,0\C,7,B8,4,A7,1,D6,0\H,9,B9,7,A8,4,D7,0\H,9,B10,7
 ,A9,4,D8,0\C,2,B11,1,A10,3,D9,0\H,12,B12,2,A11,1,D10,0\H,12,B13,2,A12,
 1,D11,0\\B1=1.32297727\B2=1.16274778\B4=1.07541561\B5=1.07564317\B6=1.
 38602995\B7=1.07585447\B8=1.50869268\B9=1.08490538\B10=1.08898237\B11=
 1.42249318\B12=1.07938611\B13=1.08319107\A1=126.02175903\A2=124.330647
 13\A3=103.5546689\A4=91.6275521\A5=94.44779426\A6=118.98303039\A7=120.
 20057822\A8=109.33138742\A9=112.40285854\A10=118.1119395\A11=105.05614
 067\A12=109.12148833\D1=-156.65710791\D2=0.26839656\D3=-116.08184168\D
 4=122.79116296\D5=-99.8066545\D6=61.13118531\D7=-149.21315858\D8=92.20
 905883\D9=-183.57789056\D10=-168.89222102\D11=-53.36930184\B3=2.198706
 31\\Version=AM64L-G09RevC.01\State=2-A\HF=-343.1338594\S2=1.029037\S2-
 1=0.\S2A=0.763345\RMSD=9.646e-09\RMSF=9.591e-05\Dipole=-1.5082365,-0.1
 196397,0.8051537\Quadrupole=-4.581611,2.756633,1.824978,-1.9877318,1.7
 619576,0.8669877\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311G(d,p)

1\1\GINC-GOMBERG12\FTS\UBHandHLYP\6-311G(d,p)\C5H7O2(2)\AHANCOCK\28-Ma
 r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/6-311G** freq=noraman
 opt=(grad,nofreeze,ts,noeigentest,readfc)\\Benchmark\\0,2\C\O,1,B1\O,1
 ,B2,2,A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\C,4,

B6,1,A5,3,D4,0\H,7,B7,4,A6,1,D5,0\C,7,B8,4,A7,1,D6,0\H,9,B9,7,A8,4,D7,
0\H,9,B10,7,A9,4,D8,0\C,2,B11,1,A10,3,D9,0\H,12,B12,2,A11,1,D10,0\H,12
,B13,2,A12,1,D11,0\\B1=1.33334785\B2=1.17158318\B4=1.07616279\B5=1.076
07635\B6=1.35788843\B7=1.07682884\B8=1.49860117\B9=1.08574172\B10=1.08
998246\B11=1.4265446\B12=1.08103831\B13=1.08466078\A1=125.3019473\A2=1
23.96902602\A3=103.359752\A4=89.02301836\A5=94.07862378\A6=119.2061297
2\A7=120.71288294\A8=109.43632663\A9=112.81846264\A10=117.34679239\A11
=105.02150085\A12=109.1727386\D1=-151.54739274\D2=-4.33370638\D3=-119.
95861161\D4=118.49864886\D5=-100.60867186\D6=62.67352582\D7=-150.42087
024\D8=90.93566853\D9=-179.97917937\D10=-168.12963702\D11=-52.46777366
\B3=2.20193192\\Version=AM64L-G09RevC.01\State=2-A\HF=-344.9785481\S2=
0.821459\S2-1=0.\S2A=0.750813\RMSD=4.789e-09\RMSF=1.791e-05\Dipole=-1.
3771136,-0.1869459,0.7844998\Quadrupole=-3.9969699,2.2181036,1.7788663
,-2.1595003,1.4294926,0.8394739\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG13\FTS\UBHandHLYP\6-311++G(d,p)\C5H7O2(2)\AHANCOCK\28-
Mar-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/6-311++G** freq=nora
man opt=(grad,nofreeze,ts,noeigentest,readfc)\\Benchmark\\0,2\C\O,1,B1
\O,1,B2,2,A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\
C,4,B6,1,A5,3,D4,0\H,7,B7,4,A6,1,D5,0\C,7,B8,4,A7,1,D6,0\H,9,B9,7,A8,4
,D7,0\H,9,B10,7,A9,4,D8,0\C,2,B11,1,A10,3,D9,0\H,12,B12,2,A11,1,D10,0\
H,12,B13,2,A12,1,D11,0\\B1=1.33075908\B2=1.17291084\B4=1.07624557\B5=1
.07605972\B6=1.35825139\B7=1.07689071\B8=1.49845107\B9=1.08578436\B10=
1.08995599\B11=1.4280134\B12=1.08112795\B13=1.08448808\A1=125.42777694
\A2=123.69933708\A3=103.49825275\A4=88.87874413\A5=93.89126233\A6=119.
19515553\A7=120.76969934\A8=109.46800692\A9=112.73569753\A10=117.49947
319\A11=104.96554869\A12=109.05347134\D1=-151.67110022\D2=-4.64076506\
D3=-120.27258042\D4=118.13875028\D5=-100.84330696\D6=62.67638399\D7=-1
50.40721524\D8=90.99830541\D9=-179.31320903\D10=-168.73425271\D11=-53.
11268038\B3=2.20180016\\Version=AM64L-G09RevC.01\State=2-A\HF=-344.985
8893\S2=0.819177\S2-1=0.\S2A=0.750776\RMSD=4.692e-09\RMSF=2.729e-05\Di
pole=-1.4891956,-0.2237651,0.8245181\Quadrupole=-4.3556745,2.4118431,1
.9438315,-2.3059795,1.5061681,0.8486033\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-GOMBERG19\FTS\UBHandHLYP\CC-pVDZ\C5H7O2(2)\AHANCOCK\01-Apr-20
13\1\\#P Geom=AllCheck Guess=Read BHandHLYP/cc-pVDZ freq=noraman opt=(
grad,nofreeze,ts,noeigentest,readfc)\\Benchmark\\0,2\C\O,1,B1\O,1,B2,2
,A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\C,4,B6,1,
A5,3,D4,0\H,7,B7,4,A6,1,D5,0\C,7,B8,4,A7,1,D6,0\H,9,B9,7,A8,4,D7,0\H,9
,B10,7,A9,4,D8,0\C,2,B11,1,A10,3,D9,0\H,12,B12,2,A11,1,D10,0\H,12,B13,
2,A12,1,D11,0\\B1=1.33758002\B2=1.17669386\B4=1.08476985\B5=1.08419051
\B6=1.36189449\B7=1.08550816\B8=1.49978464\B9=1.09383658\B10=1.0981504
5\B11=1.42515728\B12=1.08968504\B13=1.09324267\A1=124.90977152\A2=124.
29923031\A3=103.66212357\A4=88.25681727\A5=93.97337368\A6=119.09843503
\A7=120.78691014\A8=109.39411425\A9=112.90134772\A10=117.03969556\A11=
105.06225856\A12=109.34255358\D1=-151.57131522\D2=-4.33145537\D3=-119.
92537551\D4=118.57551655\D5=-101.02913413\D6=62.17447654\D7=-150.03056
647\D8=91.50881577\D9=-180.13392891\D10=-167.85724071\D11=-52.40039881
\B3=2.21280354\\Version=AM64L-G09RevC.01\State=2-A\HF=-344.9097005\S2=
0.822416\S2-1=0.\S2A=0.750827\RMSD=7.333e-09\RMSF=9.116e-05\Dipole=-1.
3235876,-0.1800973,0.7547415\Quadrupole=-3.8011547,2.0982559,1.7028987
,-2.0203818,1.3906935,0.796848\PG=C01 [X(C5H7O2)]\\@

BHandHYLP/aug-cc-pVDZ

1\1\GINC-GOMBERG19\FTS\UBHandHLYP\Aug-CC-pVDZ\C5H7O2(2)\AHANCOCK\01-Ap
r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/aug-cc-pVDZ freq=noram
an opt=(grad,nofreeze,ts,noeigentest,readfc)\\Benchmark\\0,2\C\O,1,B1\
O,1,B2,2,A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\C
,4,B6,1,A5,3,D4,0\H,7,B7,4,A6,1,D5,0\C,7,B8,4,A7,1,D6,0\H,9,B9,7,A8,4,
D7,0\H,9,B10,7,A9,4,D8,0\C,2,B11,1,A10,3,D9,0\H,12,B12,2,A11,1,D10,0\H
,12,B13,2,A12,1,D11,0\\B1=1.33495407\B2=1.17915418\B4=1.08186791\B5=1.
08138856\B6=1.36150763\B7=1.08265676\B8=1.49963097\B9=1.09071301\B10=1
.09498496\B11=1.43032831\B12=1.08669796\B13=1.08956044\A1=125.04386826
\A2=123.49451869\A3=103.40340319\A4=88.50144651\A5=93.4236255\A6=119.0
8416054\A7=120.92530156\A8=109.42951205\A9=112.7933948\A10=117.2055660
8\A11=104.87738882\A12=109.10220398\D1=-150.6468057\D2=-5.35236707\D3=
-121.0824402\D4=117.25649498\D5=-100.86407904\D6=62.99712807\D7=-150.8
1549647\D8=90.45475671\D9=-178.51120183\D10=-168.71304643\D11=-53.0624
8225\B3=2.20815673\\Version=AM64L-G09RevC.01\State=2-A\HF=-344.9340545
\S2=0.818377\S2-1=0.\S2A=0.750786\RMSD=6.505e-09\RMSF=2.105e-05\Dipole
=-1.4583852,-0.2459844,0.8215041\Quadrupole=-4.1862159,2.3111215,1.875
0945,-2.3008577,1.5913351,0.8570262\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-GOMBERG19\FTS\UBHandHLYP\CC-pVTZ\C5H7O2(2)\AHANCOCK\02-Apr-20
13\1\\#P Geom=AllCheck Guess=Read BHandHLYP/cc-pVTZ freq=noraman opt=(
grad,nofreeze,ts,noeigentest,readfc)\\Benchmark\\0,2\C\O,1,B1\O,1,B2,2
,A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\C,4,B6,1,
A5,3,D4,0\H,7,B7,4,A6,1,D5,0\C,7,B8,4,A7,1,D6,0\H,9,B9,7,A8,4,D7,0\H,9
,B10,7,A9,4,D8,0\C,2,B11,1,A10,3,D9,0\H,12,B12,2,A11,1,D10,0\H,12,B13,
2,A12,1,D11,0\\B1=1.32937802\B2=1.1719041\B4=1.07369046\B5=1.07347294\
B6=1.35403499\B7=1.07444493\B8=1.49523919\B9=1.08345976\B10=1.0876336\
B11=1.42436097\B12=1.07922667\B13=1.0823311\A1=125.32839418\A2=123.735
14215\A3=103.37763404\A4=88.80503693\A5=93.94355092\A6=119.1978056\A7=
120.79649057\A8=109.46569605\A9=112.84514217\A10=117.53755651\A11=105.
12594456\A12=109.19338023\D1=-151.27210894\D2=-5.09645816\D3=-120.6879
0261\D4=117.73410082\D5=-100.68255325\D6=62.73674459\D7=-150.34075933\
D8=91.08003919\D9=-178.95037384\D10=-168.79239134\D11=-53.12360624\B3=
2.19603451\\Version=AM64L-G09RevC.01\State=2-A\HF=-345.0159172\S2=0.81
8544\S2-1=0.\S2A=0.750783\RMSD=7.032e-09\RMSF=2.568e-05\Dipole=-1.3790
49,-0.2135944,0.8088482\Quadrupole=-3.9369368,2.1751564,1.7617804,-2.1
64081,1.5300654,0.8387765\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/aug-cc-pVTZ

1\1\GINC-GOMBERG11\FTS\UBHandHLYP\Aug-CC-pVTZ\C5H7O2(2)\AHANCOCK\02-Ap
r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/aug-cc-pVTZ freq=noram
an opt=(grad,nofreeze,ts,noeigentest,readfc)\\Benchmark\\0,2\C\O,1,B1\
O,1,B2,2,A1\C,1,B3,3,A2,2,D1,0\H,4,B4,1,A3,3,D2,0\H,4,B5,1,A4,3,D3,0\C
,4,B6,1,A5,3,D4,0\H,7,B7,4,A6,1,D5,0\C,7,B8,4,A7,1,D6,0\H,9,B9,7,A8,4,
D7,0\H,9,B10,7,A9,4,D8,0\C,2,B11,1,A10,3,D9,0\H,12,B12,2,A11,1,D10,0\H
,12,B13,2,A12,1,D11,0\\B1=1.32844406\B2=1.1720519\B4=1.07362081\B5=1.0
7340314\B6=1.35395585\B7=1.07437883\B8=1.49509074\B9=1.08333602\B10=1.
08744325\B11=1.42549814\B12=1.07906991\B13=1.08214875\A1=125.41274406\
A2=123.53909927\A3=103.39329519\A4=88.79776505\A5=93.81213614\A6=119.1
9153587\A7=120.82710246\A8=109.48084786\A9=112.79717933\A10=117.591877
14\A11=105.07304636\A12=109.10593539\D1=-151.26556133\D2=-5.2510886\D3
=-120.87368268\D4=117.53838011\D5=-100.70974063\D6=62.85037804\D7=-150
.49551997\D8=90.92481189\D9=-178.6006641\D10=-169.08043759\D11=-53.419

76648\B3=2.19564103\\Version=AM64L-G09RevC.01\State=2-A\HF=-345.020737
5\S2=0.817277\S2-1=0.\S2A=0.750766\RMSD=7.667e-09\RMSF=2.666e-05\Dipol
e=-1.4360141,-0.2315956,0.8247939\Quadrupole=-4.13158,2.2965554,1.8350
246,-2.2388595,1.5773272,0.8375928\PG=C01 [X(C5H7O2]\\@

ROMP2/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.228764

QCISD/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.277337

CCSD(T)/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.320300

ROMP2/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.230506

QCISD/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.278348

CCSD(T)/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.322021

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.164575

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.217882

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.2591401

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.167468

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.219909

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.322021

B3LYP/6-31G(d) Gaussian Archive Entries for the higher energy endo transition states involved in the cyclization of radicals 1, 7 – 11

Transition state for the cyclization of 7 X=CH2 endo Boat

1\1\GINC-V1440\FTS\UB3LYP\Gen\C8H13O1(2)\AXH563\09-Jan-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=2684354560\\S51.freq\\0,2\C,-0.0121718074
,0.0076712451,-0.0180864036\O,-0.0129551978,0.0485422306,1.1780360063\
C,1.9514044396,0.0006491036,-1.0307727722\H,2.6025328754,0.3411233002,
-0.2308346758\H,1.6313622498,0.7699660901,-1.7271816384\C,1.8481621765
,-1.3254720804,-1.3345151354\H,2.3304771089,-2.053743189,-0.6857211065
\C,0.8681212424,-1.8275959467,-2.3640863766\H,0.6595315728,-2.88868063
79,-2.1856682111\H,1.2817014662,-1.7724836363,-3.3828725369\C,-0.44568
8948,-1.0122248389,-2.3188317855\H,-1.2092989803,-1.5131369146,-2.9280
402568\H,-0.281410303,-0.0322983986,-2.7843855092\C,-1.012568656,-0.78
58276201,-0.9006435094\C,-1.3722361464,-2.1091752817,-0.1974333427\H,-
1.7579899529,-1.9127767411,0.8070625893\H,-2.1395252793,-2.6480621506,
-0.767630285\H,-0.5001729647,-2.7628737513,-0.0950177613\C,-2.26685185
98,0.1142905922,-0.9898182775\H,-2.0343025411,1.0783236119,-1.45626524
39\H,-3.038632099,-0.3789020288,-1.5922268671\H,-2.6790578213,0.308109
483,0.0056560121\\Version=EM64L-G09RevA.02\State=2-A\HF=-387.8127197\S
2=0.769584\S2-1=0.\S2A=0.75009\RMSD=7.338e-09\RMSF=1.634e-05\Dipole=-0
.2075566,-0.342202,-0.9091588\Quadrupole=1.7466225,1.2483102,-2.994932
7,-0.1017083,0.3370937,-1.7135558\PG=C01 [X(C8H13O1)]\\@

Transition state for the cyclization of 8 X=CH2 endo Boat

1\1\GINC-V1365\FTS\UB3LYP\Gen\C8H13O1(2)\AXH563\01-May-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=1342177280\\S56.freq\\0,2\C,0.0104089096,
0.0916739954,-0.0208112655\O,-0.1071642157,0.1722336394,1.1677336298\C
,2.0655058007,-0.1241397903,-0.7844080214\H,2.6106352455,0.0179242437,
0.1445645926\H,2.0200137636,0.7457755923,-1.431555291\C,1.7916679822,-
1.3780537644,-1.2463714935\H,2.0086233763,-2.2256330869,-0.5987301839\
C,0.9265276586,-1.633428638,-2.4524123071\H,0.7247175231,-2.7088387069
,-2.5183876454\H,1.4446310133,-1.3656711234,-3.3852373347\C,-0.4460422
503,-0.8636518684,-2.4139677617\C,-0.9241349818,-0.6854336539,-0.95722
24463\H,-1.8695370254,-0.1247991021,-0.9490332461\H,-1.1389179536,-1.6
559979256,-0.4869722856\C,-1.4919021106,-1.6992883738,-3.1781591177\H,
-2.460367773,-1.185940299,-3.2189091466\H,-1.1657792726,-1.8766596999,
-4.2102829544\H,-1.6474734943,-2.6757940295,-2.704149712\C,-0.33858180
3,0.5142911454,-3.0990112597\H,0.013091652,0.4086102961,-4.1320524819\
H,-1.3202233647,1.0035276488,-3.1299321792\H,0.3441172944,1.1896887441
,-2.576499686\\Version=EM64L-G09RevA.02\State=2-A\HF=-387.8082084\S2=0
.770322\S2-1=0.\S2A=0.750094\RMSD=5.402e-09\RMSF=1.044e-05\Dipole=-0.1
123498,-0.3673973,-0.99304\Quadrupole=2.2190494,2.0037342,-4.2227835,0
.246415,1.0126507,-2.2481723\PG=C01 [X(C8H13O1)]\\@

Transition state for the cyclization of 9 X=CH2 endo Boat

1\1\GINC-V1427\FTS\UB3LYP\Gen\C8H13O1(2)\AXH563\09-Jan-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=2684354560\\S52.freq\\0,2\C,0.0103530373,
0.0583509621,-0.0090069619\O,0.0289798122,0.1115088357,1.1855756105\C,
1.9409650173,-0.0112666495,-1.0950949961\H,2.6219805323,0.3423508453,-
0.3263997634\H,1.610028584,0.7429306957,-1.802952693\C,1.8050873091,-1
.3438513116,-1.3489176817\H,2.2930948521,-2.0559437253,-0.6849011508\C
,0.8121281667,-1.8944439334,-2.3579688589\C,-0.4802197093,-1.026506540
1,-2.2942392422\H,-1.2781354729,-1.5253465473,-2.8590962002\H,-0.30018
9803,-0.0714403745,-2.8033961737\C,-0.9740676063,-0.7362505722,-0.8719
58015\H,-1.8825659199,-0.1194573576,-0.915910998\H,-1.2491614943,-1.65
31388788,-0.3324384716\C,1.3863248428,-1.8345663453,-3.7917838669\H,2.
2824023713,-2.4589820264,-3.881549901\H,0.6492228695,-2.1926117583,-4.
5224867922\H,1.6638304611,-0.8097264904,-4.06265336\C,0.4897282854,-3.
3607490856,-2.0076029953\H,-0.2218619317,-3.7886668851,-2.7236289726\H
,1.4000234635,-3.9718164708,-2.0337933295\H,0.0594394024,-3.4561447176
,-1.0040988637\\Version=EM64L-G09RevA.02\State=2-A\HF=-387.8122924\S2=
0.768991\S2-1=0.\S2A=0.750085\RMSD=4.343e-09\RMSF=2.481e-05\Dipole=-0.
1561227,-0.3742844,-0.9667855\Quadrupole=3.0992228,1.467955,-4.5671778
,0.0316711,1.4306186,-2.8943437\PG=C01 [X(C8H13O1)]\\@

Transition state for the cyclization of 10 X=CH2 endo Boat

1\1\GINC-V1422\FTS\UB3LYP\Gen\C7H11O1(2)\AXH563\08-Jan-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=4026531840\\S50.freq\\0,2\C,-0.0025177947
,-0.0092422396,0.0019784462\O,0.0258226338,-0.0732488799,1.1982000612\
C,1.9121050285,0.021706073,-1.0660601563\H,2.5812846035,0.4010414889,-
0.298694794\H,1.5577894623,0.7597275961,-1.7781956142\C,1.8378780966,-
1.3193741333,-1.3251979951\C,0.8409812275,-1.830330786,-2.3454994266\H
,0.5911848342,-2.8740857697,-2.1094886423\H,1.268585329,-1.8463535551,
-3.3595347327\C,-0.4524793779,-0.9878139858,-2.3385847844\H,-1.2240375
709,-1.485496875,-2.9378606435\H,-0.2729467413,-0.0171862498,-2.816029
2899\C,-0.9762806413,-0.7598038157,-0.9155889023\H,-1.8887800163,-0.14
86455927,-0.9419626869\H,-1.2468045736,-1.7105513609,-0.4314792423\C,2
.5358213433,-2.3328764473,-0.4629157161\H,3.0999832224,-3.0497460521,-
1.0764931755\H,3.2333683449,-1.8632737316,0.2371460529\H,1.8154392311,
-2.9247473503,0.1225323292\\Version=EM64L-G09RevA.02\State=2-A\HF=-348
.5047969\S2=0.768358\S2-1=0.\S2A=0.750082\RMSD=9.859e-09\RMSF=3.132e-0
6\Dipole=-0.0534541,-0.4096566,-1.0353093\Quadrupole=2.385907,1.134051
2,-3.5199582,-0.0077377,1.9755762,-1.8368161\PG=C01 [X(C7H11O1)]\\@

Transition state for the cyclization of 1 X=CH2 endo Boat

1\1\GINC-V1466\FTS\UB3LYP\Gen\C6H9O1(2)\AXH563\08-Jan-2013\0\\#B3LYP/g
en 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(2
/17=4) Freq=noraman maxdisk=5368709120\\S49.freq\\0,2\C,0.111310179,-0
.0509427952,0.1003939819\O,0.3062562844,-0.2839905397,1.2572130865\C,1
.8428628576,0.067443396,-1.2626978947\H,2.6622839365,0.2207687421,-0.5
664108227\H,1.4527666398,0.9698358687,-1.7236668458\C,1.5891233278,-1.
1701254498,-1.7802295402\H,2.1373939163,-2.0246104335,-1.388916879\C,0

.3950189513,-1.4420907635,-2.6606839444\H,0.1088515745,-2.4976456118,-
2.5630250155\H,0.6244413672,-1.2908231639,-3.7268472996\C,-0.800501707
8,-0.5499908499,-2.2603529256\H,-1.7039571583,-0.8805077721,-2.7862752
281\H,-0.6210805986,0.4834676885,-2.5804931022\C,-1.0551013797,-0.5699
965785,-0.7484359226\H,-1.9060729489,0.0794232531,-0.5008205351\H,-1.3
169656677,-1.5792143496,-0.3976175492\\Version=EM64L-G09RevA.02\State=
2-A\HF=-309.1846054\S2=0.769993\S2-1=0.\S2A=0.750091\RMSD=6.037e-09\RM
SF=1.161e-05\Dipole=-0.3588693,-0.1170961,-0.9916076\Quadrupole=2.3526
012,1.9903907,-4.3429919,-0.206847,0.3415431,-0.5085943\PG=C01 [X(C6H9
O1)]\\@

Transition state for the cyclization of 11 X=CH2 endo Boat

1\1\GINC-V1429\FTS\UB3LYP\Gen\C8H13O1(2)\AXH563\09-Jan-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=2684354560\\S53.freq\\0,2\C,-0.0371373543
,0.0313250064,-0.1173546885\O,-0.0416575515,0.2388201217,1.0652752033\
C,1.8921364315,0.0848704598,-1.0553952045\C,1.7391345052,-1.2558125584
,-1.3591471033\H,2.1216414009,-1.9745507197,-0.6365234123\C,0.81870825
18,-1.7902571991,-2.4255561922\H,0.7591754131,-2.8796626268,-2.3214394
581\H,1.2017243484,-1.603670032,-3.4395661117\C,-0.6095950121,-1.18427
4679,-2.3078568874\H,-1.3388463849,-1.8660368095,-2.7606730224\H,-0.67
16901317,-0.2511236256,-2.8772147448\C,-1.0038390928,-0.8982462249,-0.
8576189299\H,-1.982931479,-0.4018762575,-0.8193101901\H,-1.1026346624,
-1.8234946103,-0.2714482456\C,2.7736431723,0.4780110867,0.1114062365\H
,3.7399225541,0.853350595,-0.2504573971\H,2.3045507445,1.2714979652,0.
702583866\H,2.9611205027,-0.3671296511,0.7803982302\C,1.7245908108,1.1
886049297,-2.0861722688\H,2.7080146872,1.4285000071,-2.516277583\H,1.0
659824441,0.9145758204,-2.912273646\H,1.3375655234,2.1040648691,-1.627
0365281\\Version=EM64L-G09RevA.02\State=2-A\HF=-387.8164688\S2=0.77297
6\S2-1=0.\S2A=0.750109\RMSD=6.336e-09\RMSF=1.375e-05\Dipole=-0.0485471
,-0.3368068,-0.9120129\Quadrupole=1.9282363,1.5850494,-3.5132856,1.371
8128,2.1018077,-1.4368576\PG=C01 [X(C8H13O1)]\\@

Transition state for the cyclization of 1 X=O endo Chair

1\1\GINC-GOMBERG19\FTS\UB3LYP\6-31G(d)\C5H7O2(2)\CARLHS\06-Jan-2014\1\
\#b3lyp/6-31g* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoi
nt guess=read\\Oxyacyl radical endo transition state\\0,2\C\O,1,B1\C,1
,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,
B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,
0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\O,1
,B13,2,A12,3,D11,0\\B1=1.19433943\B3=1.08645844\B4=1.08870809\B5=1.365
69821\B6=1.08899446\B7=1.49838063\B8=1.09647397\B9=1.09711352\B10=1.54
346723\B11=1.09313891\B12=1.09567612\B13=1.35589548\A1=120.18610554\A2
=105.2318062\A3=80.48605403\A4=101.04756381\A5=119.50505953\A6=118.919
61754\A7=112.63453987\A8=111.85925109\A9=107.79462823\A10=111.19738155
\A11=110.6082583\A12=123.53857751\D1=49.39357046\D2=-63.95221577\D3=17
6.77636693\D4=-105.28669193\D5=51.3591143\D6=-190.06258154\D7=48.35929
299\D8=-70.82063628\D9=-177.62407877\D10=-56.9304219\D11=219.64884742\
B2=2.21897077\\Version=AM64L-G09RevC.01\State=2-A\HF=-345.0903728\S2=0
.779358\S2-1=0.\S2A=0.750157\RMSD=8.391e-09\RMSF=4.251e-05\Dipole=0.11
73037,0.025977,-1.5014182\Quadrupole=1.261541,1.8260968,-3.0876378,-0.

0993871,2.8834975,0.5549654\PG=C01 [X(C5H7O2)]\\@

Transition state for the cyclization of 8 X=O endo Chair

1\1\GINC-GOMBERG19\FTS\UB3LYP\6-31G(d)\C7H11O2(2)\CARLHS\10-Jan-2014\1
\\#b3lyp/6-31g* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpo
int guess=read\\3,3-dimethyl oxyacyl radical endo transition state\\0,
2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,
A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8
,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\C,11,B11,8,A10,6,D9,0\C,11,B12,8,A
11,6,D10,0\O,1,B13,2,A12,3,D11,0\H,12,B16,11,A15,8,D14,0\H,12,B17,11,A
16,8,D15,0\H,12,B18,11,A17,8,D16,0\H,13,B19,11,A18,8,D17,0\H,13,B20,11
,A19,8,D18,0\H,13,B21,11,A20,8,D19,0\\B1=1.19572275\B3=1.08657172\B4=1
.08860833\B5=1.36450421\B6=1.0880665\B7=1.49673633\B8=1.09618502\B9=1.
09741822\B10=1.56067971\B11=1.52911584\B12=1.53054424\B13=1.35134498\B
16=1.09434908\B17=1.0951056\B18=1.09459937\B19=1.09463441\B20=1.093949
37\B21=1.0958053\A1=119.90148311\A2=105.93034281\A3=79.71083342\A4=100
.5717278\A5=119.63289883\A6=118.8073108\A7=112.2587019\A8=111.09225784
\A9=110.54309003\A10=110.28974461\A11=112.49806884\A12=123.72503242\A1
5=110.47314266\A16=110.15778902\A17=110.70451901\A18=110.12216199\A19=
111.21224401\A20=110.43763191\D1=47.79508582\D2=-65.30391088\D3=175.40
975962\D4=-107.4935008\D5=51.60831155\D6=-191.4716282\D7=48.1372378\D8
=-71.1128018\D9=-183.51390389\D10=-58.52906832\D11=219.91919531\D14=18
3.15646118\D15=63.21161233\D16=-56.87358401\D17=179.97302998\D18=59.98
180114\D19=-60.37249045\B2=2.22281547\\Version=AM64L-G09RevC.01\State=
2-A\HF=-423.7259237\S2=0.7788\S2-1=0.\S2A=0.750155\RMSD=5.023e-09\RMSF
=2.539e-05\Dipole=-0.0359535,0.0114531,-1.5362862\Quadrupole=2.3711505
,2.3569287,-4.7280792,-0.08508,1.5965062,0.6424382\PG=C01 [X(C7H11O2)]
\\@

Transition state for the cyclization of 9 X=O endo Chair

1\1\GINC-GOMBERG19\FTS\UB3LYP\6-31G(d)\C7H11O2(2)\CARLHS\10-Jan-2014\1
\\#b3lyp/6-31g* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpo
int guess=read\\4,4-dimethyl oxyacyl radical endo transition state\\0,
2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,
A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\C,8,B8,6,A7,3,D6,0\C,8
,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A
11,6,D10,0\O,1,B13,2,A12,3,D11,0\H,9,B16,8,A15,11,D14,0\H,9,B17,8,A16,
11,D15,0\H,9,B18,8,A17,11,D16,0\H,10,B19,8,A18,11,D17,0\H,10,B20,8,A19
,11,D18,0\H,10,B21,8,A20,11,D19,0\\B1=1.19465285\B3=1.08654058\B4=1.08
720504\B5=1.36553691\B6=1.09016926\B7=1.51128782\B8=1.53933799\B9=1.53
989675\B10=1.5564956\B11=1.09434835\B12=1.0958266\B13=1.35592122\B16=1
.095413\B17=1.09614691\B18=1.09695321\B19=1.09510184\B20=1.09351141\B2
1=1.09652368\A1=120.27025083\A2=105.42197838\A3=80.74362495\A4=101.053
96581\A5=118.46683561\A6=121.60559246\A7=110.80471459\A8=113.62746283\
A9=104.53633174\A10=110.53862782\A11=110.22569695\A12=123.56906175\A15
=110.28986898\A16=111.27120128\A17=111.51168372\A18=110.3970865\A19=11
2.20602569\A20=110.36935842\D1=51.69136077\D2=-61.35212447\D3=178.2767
435\D4=-105.32390439\D5=51.55196709\D6=-184.83930706\D7=50.85949526\D8
=-69.18198886\D9=-177.73948354\D10=-57.79458949\D11=221.17942278\D14=1
81.26754165\D15=61.60052176\D16=-59.10902145\D17=177.52718806\D18=56.7
060623\D19=-62.98939518\B2=2.21082921\\Version=AM64L-G09RevC.01\State=

2-A\HF=-423.7183069\S2=0.778706\S2-1=0.\S2A=0.750152\RMSD=6.809e-09\RM
SF=3.436e-05\Dipole=0.1600383,0.0731592,-1.5371445\Quadrupole=2.374451
9,2.778983,-5.1534349,-0.1149313,2.8615095,1.3209335\PG=C01 [X(C7H11O2
)]\\@

Transition state for the cyclization of 10 X=O endo Chair

1\1\GINC-GOMBERG19\FTS\UB3LYP\6-31G(d)\C6H9O2(2)\CARLHS\10-Jan-2014\1\
\#b3lyp/6-31g* opt=(grad,ts,noeigentest,readfc,nofreeze) geom=checkpoi
nt guess=read\\5_Methyl oxyacyl radical endo transition state\\0,2\C\O
,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,
D3,0\C,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6
,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,
D10,0\O,1,B13,2,A12,3,D11,0\H,7,B19,6,A18,3,D17,0\H,7,B20,6,A19,3,D18,
0\H,7,B21,6,A20,3,D19,0\\B1=1.19521707\B3=1.08701117\B4=1.08793053\B5=
1.3692407\B6=1.50187534\B7=1.50534016\B8=1.09722758\B9=1.09658068\B10=
1.54399488\B11=1.09288011\B12=1.09619087\B13=1.35957666\B19=1.09877909
\B20=1.10198326\B21=1.09415846\A1=119.88919531\A2=104.79531279\A3=80.8
9872226\A4=101.76695359\A5=122.53410068\A6=116.41037039\A7=112.4266325
7\A8=111.90648055\A9=108.05969373\A10=111.05591673\A11=110.57906149\A1
2=123.13373231\A18=111.03474535\A19=111.75007609\A20=111.7626668\D1=47
.81886939\D2=-65.71383701\D3=175.09224412\D4=-106.14941938\D5=53.61993
324\D6=-190.50875741\D7=48.06977941\D8=-71.31485371\D9=-177.45988458\D
10=-57.07228538\D11=222.19419443\D17=225.99737702\D18=107.49623546\D19
=-13.2570623\B2=2.19934657\\Version=AM64L-G09RevC.01\State=2-A\HF=-384
.4107371\S2=0.77751\S2-1=0.\S2A=0.750146\RMSD=3.803e-09\RMSF=1.357e-05
\Dipole=0.2174646,-0.0284289,-1.6517603\Quadrupole=1.7764897,2.3109592
,-4.0874489,-0.179884,3.0471867,-0.0401796\PG=C01 [X(C6H9O2)]\\@

Transition state for the cyclization of 11 X=O endo Chair

1\1\GINC-V1410\FTS\UB3LYP\Gen\C8H13O2(2)\AXH563\08-Jan-2013\0\\#B3LYP/
gen 6D INT(grid=ultrafine) OPT=(TS,calcfc,noeigentest,maxcyc=200) IOP(
2/17=4) Freq=noraman maxdisk=4026531840\\S33-2.freq\\0,2\C,-0.01001805
,-0.0590062406,-0.040214144\O,0.0250123889,0.014270506,1.3157818353\O,
0.9798339279,-0.0286071139,-0.7145112274\C,-1.8286724437,0.9606166561,
-0.7849338553\C,-2.6871275095,0.4946615561,0.204577019\C,-2.335370484,
0.7553659616,1.6458082263\H,-3.1850476944,0.5571011108,2.311160551\H,-
2.0122671888,1.7828948776,1.8352510077\C,-1.1956475225,-0.2045120984,2
.0497216112\H,-1.5066002371,-1.247488135,1.9196710436\H,-0.9090720445,
-0.0590050093,3.0945989028\C,-1.162874138,2.3315197127,-0.7050079046\H
,-0.2114420642,2.3346671448,-1.2441176534\H,-1.8195466406,3.0666163909
,-1.1911848587\H,-0.9735431511,2.6753886268,0.3130657148\C,-1.93064282
16,0.4664388852,-2.2135681301\H,-2.591928806,1.1167163069,-2.803441966
7\H,-0.9406578872,0.4939308916,-2.6800991599\H,-2.3040093203,-0.557143
9538,-2.2858013659\C,-3.6227416675,-0.6637706713,-0.0390943249\H,-4.38
42422808,-0.7199052649,0.7469269503\H,-4.1426800545,-0.5851666205,-0.9
983095463\H,-3.0939350811,-1.6327848344,-0.041277724\\Version=EM64L-G0
9RevA.02\State=2-A\HF=-463.0387153\S2=0.784175\S2-1=0.\S2A=0.750191\RM
SD=5.048e-09\RMSF=2.342e-06\Dipole=-1.3962933,0.1236884,0.559815\Quadr
upole=-5.7067656,2.0389635,3.6678022,1.8771637,0.8003932,-1.2289112\PG
=C01 [X(C8H13O2)]\\@

Gaussian Archive Entries for higher energy endo transition states 3 at all levels of theory used in this study

Transition State 3 X=O endo Chair

HF/6-31G(d)

1\1\GINC-GOMBERG19\FTS\UHF\6-31G(d)\C5H7O2(2)\CARLHS\06-Jan-2014\1\\#U
HF/6-31G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoint gu
ess=read\\Oxyacyl radical endo transition state\\0,2\C\O,1,B1\C,1,B2,2
,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,B6,3,
A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,0\C,8
,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\O,1,B13,
2,A12,3,D11,0\\B1=1.16986804\B3=1.07511022\B4=1.07737234\B5=1.38637171
\B6=1.07731873\B7=1.50181936\B8=1.08546345\B9=1.08595903\B10=1.5309037
4\B11=1.07979268\B12=1.08354336\B13=1.32392097\A1=121.08204306\A2=105.
58892004\A3=83.4175583\A4=100.32453062\A5=119.28411573\A6=117.97791204
\A7=111.9039987\A8=111.25444544\A9=108.79661196\A10=111.22956928\A11=1
10.55431593\A12=125.33963701\D1=43.43506917\D2=-70.7993557\D3=170.0915
1074\D4=-103.88098051\D5=50.4231868\D6=-190.31029725\D7=49.2087261\D8=
-70.90563589\D9=-178.49129102\D10=-58.08332025\D11=209.50266876\B2=2.2
0199123\\Version=AM64L-G09RevC.01\State=2-A\HF=-343.0473972\S2=1.04917
3\S2-1=0.\S2A=0.765139\RMSD=5.871e-09\RMSF=6.750e-06\Dipole=0.1764238,
-0.1274938,-1.6945413\Quadrupole=1.5954837,2.506603,-4.1020867,0.22278
02,3.2331996,0.4267096\PG=C01 [X(C5H7O2)]\\@

HF/6-311G(d,p)

1\1\GINC-GOMBERG19\FTS\UHF\6-311G(d,p)\C5H7O2(2)\CARLHS\06-Jan-2014\1\
\#UHF/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoi
nt guess=read\\Oxyacyl radical endo transition state\\0,2\C\O,1,B1\C,1
,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,
B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,
0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\O,1
,B13,2,A12,3,D11,0\\B1=1.16313613\B3=1.07558211\B4=1.07783813\B5=1.386
15916\B6=1.07795451\B7=1.50151625\B8=1.08562422\B9=1.08640693\B10=1.53
00248\B11=1.08001225\B12=1.08466284\B13=1.32156143\A1=121.0085933\A2=1
05.51036603\A3=83.20890091\A4=100.67434961\A5=119.27896136\A6=117.8208
7372\A7=111.90399891\A8=111.19220091\A9=108.79127422\A10=111.18162407\
A11=110.50436917\A12=125.57993446\D1=42.85836879\D2=-71.47024509\D3=16
9.55923628\D4=-104.09618857\D5=50.1692432\D6=-189.90276077\D7=49.51446
432\D8=-70.61758287\D9=-178.59178085\D10=-58.18692967\D11=208.46665391
\B2=2.19125097\\Version=AM64L-G09RevC.01\State=2-A\HF=-343.1330254\S2=
1.040572\S2-1=0.\S2A=0.764491\RMSD=6.162e-09\RMSF=1.501e-05\Dipole=0.1
490585,-0.1242312,-1.6632042\Quadrupole=1.4452679,2.5602693,-4.0055372
,0.2178596,3.3229148,0.4071882\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311G(d,p)

1\1\GINC-GOMBERG19\FTS\UBHandHLYP\6-311G(d,p)\C5H7O2(2)\CARLHS\06-Jan-
2014\1\\#bhandhlyp/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze)
geom=checkpoint guess=read\\Oxyacyl radical endo transition state\\0,2
\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A
4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,
B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A1
1,6,D10,0\O,1,B13,2,A12,3,D11,0\\B1=1.17240157\B3=1.07626954\B4=1.0788
4531\B5=1.35811522\B6=1.07856454\B7=1.49056156\B8=1.08600761\B9=1.0870

1323\B10=1.52857742\B11=1.08201547\B12=1.08572485\B13=1.33208388\A1=12
0.51665457\A2=105.20569694\A3=80.4798197\A4=101.18046023\A5=119.643614
21\A6=118.50235782\A7=112.46000799\A8=111.56739447\A9=107.84210252\A10
=111.25760934\A11=110.56735615\A12=124.65625993\D1=46.59231788\D2=-67.
06235146\D3=173.88520421\D4=-105.83369084\D5=51.20563034\D6=-190.25616
705\D7=48.36538344\D8=-71.01180516\D9=-178.12822403\D10=-57.48065896\D
11=215.04082231\B2=2.18156057\\Version=AM64L-G09RevC.01\State=2-A\HF=-
344.977223\S2=0.826479\S2-1=0.\S2A=0.750889\RMSD=8.139e-09\RMSF=2.400e
-05\Dipole=0.1082359,-0.0326075,-1.5580159\Quadrupole=1.1883031,2.1486
476,-3.3369507,-0.0182263,3.1894797,0.5189977\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\6-311++G(d,p)\C5H7O2(2)\CARLHS\06-Ja
n-2014\1\\#bhandhlyp/6-311++G** opt=(grad,ts,readfc,noeigentest,nofree
ze) geom=checkpoint guess=read\\Oxyacyl radical endo transition state\
\0,2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5
,1,A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\
H,8,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,
8,A11,6,D10,0\O,1,B13,2,A12,3,D11,0\\B1=1.17363444\B3=1.07631095\B4=1.
0788882\B5=1.35846111\B6=1.07858524\B7=1.49032481\B8=1.08603382\B9=1.0
8703801\B10=1.52812107\B11=1.08207299\B12=1.08562175\B13=1.32955629\A1
=120.26339041\A2=105.19790826\A3=80.54860891\A4=100.85405462\A5=119.64
3317\A6=118.5573104\A7=112.40807255\A8=111.56984551\A9=107.93657252\A1
0=111.25442173\A11=110.69332473\A12=124.78176905\D1=46.42775362\D2=-67
.32933762\D3=173.53901194\D4=-105.90178899\D5=51.4930758\D6=-190.44609
983\D7=48.25121596\D8=-71.34607977\D9=-178.53171094\D10=-57.77287126\D
11=214.65308408\B2=2.18247168\\Version=AM64L-G09RevC.01\State=2-A\HF=-
344.9846488\S2=0.823932\S2-1=0.\S2A=0.750841\RMSD=4.917e-09\RMSF=2.695
e-05\Dipole=0.1405672,-0.0430987,-1.675091\Quadrupole=1.2286524,2.3486
729,-3.5773253,0.0386575,3.4695671,0.4742471\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\CC-pVDZ\C5H7O2(2)\CARLHS\06-Jan-2014
\1\\#bhandhlyp/cc-pVDZ opt=(grad,ts,readfc,noeigentest,nofreeze) geom=
checkpoint guess=read\\Oxyacyl radical endo transition state\\0,2\C\O,
1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D
3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,
A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D
10,0\O,1,B13,2,A12,3,D11,0\\B1=1.17733333\B3=1.08475113\B4=1.0867372\B
5=1.36210312\B6=1.08704175\B7=1.4919776\B8=1.09370614\B9=1.09506641\B1
0=1.52828893\B11=1.0903557\B12=1.09419963\B13=1.33660998\A1=120.666807
46\A2=105.41655427\A3=80.09948999\A4=101.03081803\A5=119.54394164\A6=1
18.54255846\A7=112.48044655\A8=111.59753047\A9=107.90395379\A10=111.18
906706\A11=110.50379147\A12=124.29536524\D1=46.72042973\D2=-66.9528833
7\D3=174.09064956\D4=-105.84706168\D5=51.05853206\D6=-190.01860832\D7=
48.64554406\D8=-70.71908842\D9=-177.66928602\D10=-57.38387586\D11=215.
79203765\B2=2.18907251\\Version=AM64L-G09RevC.01\State=2-A\HF=-344.908
4127\S2=0.827966\S2-1=0.\S2A=0.750915\RMSD=8.930e-09\RMSF=2.955e-05\Di
pole=0.1041274,-0.0184933,-1.4915542\Quadrupole=1.2308112,1.9921135,-3
.2229247,-0.0183224,3.0068351,0.5017682\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\Aug-CC-pVDZ\C5H7O2(2)\CARLHS\07-Jan-
2014\1\\#bhandhlyp/aug-cc-pVDZ opt=(grad,ts,readfc,noeigentest,nofreez
e) geom=checkpoint guess=read\\Oxyacyl radical endo transition state\\

0,2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,
1,A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H
,8,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8
,A11,6,D10,0\O,1,B13,2,A12,3,D11,0\\B1=1.17979547\B3=1.08189024\B4=1.0
8404386\B5=1.36186249\B6=1.08426265\B7=1.4916853\B8=1.09118528\B9=1.09
188444\B10=1.52861773\B11=1.08769653\B12=1.09088496\B13=1.33396103\A1=
119.9025226\A2=105.18186636\A3=80.08610521\A4=100.6321526\A5=119.56839
203\A6=118.6919097\A7=112.36475946\A8=111.64736673\A9=107.88127235\A10
=111.20063\A11=110.6918918\A12=124.37128615\D1=47.36558461\D2=-66.4879
2926\D3=174.35729297\D4=-106.06854889\D5=51.61238051\D6=-190.174714\D7
=48.25701964\D8=-71.3174008\D9=-178.4322423\D10=-57.5830319\D11=216.13
273743\B2=2.18466114\\Version=AM64L-G09RevC.01\State=2-A\HF=-344.93266
37\S2=0.82384\S2-1=0.\S2A=0.750864\RMSD=3.157e-09\RMSF=5.040e-05\Dipol
e=0.1352138,-0.0189148,-1.6527794\Quadrupole=1.2731666,2.2970306,-3.57
01973,-0.0556244,3.3143618,0.5102754\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-GOMBERG19\FTS\UBHandHLYP\CC-pVTZ\C5H7O2(2)\CARLHS\07-Jan-2014
\1\\#bhandhlyp/cc-pVTZ opt=(grad,ts,readfc,noeigentest,nofreeze) geom=
checkpoint guess=read\\Oxyacyl radical endo transition state\\0,2\C\O,
1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D
3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,
A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D
10,0\O,1,B13,2,A12,3,D11,0\\B1=1.17268776\B3=1.07377689\B4=1.0764601\B
5=1.35422581\B6=1.07615496\B7=1.48697918\B8=1.08362207\B9=1.08469144\B
10=1.52527792\B11=1.08019428\B12=1.08354575\B13=1.32800635\A1=120.4186
5759\A2=105.18679394\A3=80.3710498\A4=101.01346224\A5=119.63303959\A6=
118.64307484\A7=112.47991622\A8=111.60949544\A9=107.83388076\A10=111.1
5957862\A11=110.52294991\A12=124.66152233\D1=46.79284112\D2=-66.866164
86\D3=174.01025176\D4=-105.94811934\D5=51.35246175\D6=-190.38341456\D7
=48.22854332\D8=-71.25347751\D9=-178.31788977\D10=-57.84950702\D11=214
.73074749\B2=2.17729416\\Version=AM64L-G09RevC.01\State=2-A\HF=-345.01
44593\S2=0.82388\S2-1=0.\S2A=0.75086\RMSD=9.002e-09\RMSF=3.340e-05\Dip
ole=0.1018158,-0.0095678,-1.5752292\Quadrupole=1.2485026,2.1793767,-3.
4278793,-0.0547357,3.1315611,0.5265839\PG=C01 [X(C5H7O2)]\\@

BHandHLYP/aug-cc-pVTZ

1\1\GINC-GOMBERG16\FTS\UBHandHLYP\Aug-CC-pVTZ\C5H7O2(2)\CARLHS\07-Jan-
2014\1\\#bhandhlyp/aug-cc-pVTZ opt=(grad,ts,readfc,noeigentest,nofreez
e) geom=checkpoint guess=read\\Oxyacyl radical endo transition state\\
0,2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,
1,A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H
,8,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8
,A11,6,D10,0\O,1,B13,2,A12,3,D11,0\\B1=1.17275063\B3=1.07368413\B4=1.0
7639212\B5=1.35420601\B6=1.07608619\B7=1.48679198\B8=1.08345764\B9=1.0
845459\B10=1.52514339\B11=1.07999569\B12=1.08334739\B13=1.32703264\A1=
120.26922323\A2=105.1484585\A3=80.38997008\A4=100.88194793\A5=119.6333
6322\A6=118.67372632\A7=112.46800894\A8=111.60381507\A9=107.86486645\A
10=111.18542432\A11=110.59075052\A12=124.74439783\D1=46.69331367\D2=-6
7.02250205\D3=173.83284756\D4=-105.94632516\D5=51.51961523\D6=-190.451
48481\D7=48.15004833\D8=-71.38915272\D9=-178.54133126\D10=-57.95010042
\D11=214.64391157\B2=2.17704549\\Version=AM64L-G09RevC.01\State=2-A\HF
=-345.0193675\S2=0.822462\S2-1=0.\S2A=0.750837\RMSD=9.167e-09\RMSF=3.4
34e-05\Dipole=0.1178973,-0.0186051,-1.6317245\Quadrupole=1.2705617,2.2
949184,-3.5654801,-0.0153232,3.2688781,0.488136\PG=C01 [X(C5H7O2)]\\@

MP2/6-311G(d,p)

1\1\GINC-GOMBERG01\FTS\UMP2-FC\6-311G(d,p)\C5H7O2(2)\CARLHS\07-Jan-201
4\1\\#mp2=direct/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) ge
om=checkpoint guess=read\\Oxyacyl radical endo transition state\\0,2\C
\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,
2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9
,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,
6,D10,0\O,1,B13,2,A12,3,D11,0\\B1=1.18995201\B3=1.08512524\B4=1.087721
88\B5=1.35094843\B6=1.08692394\B7=1.49437368\B8=1.09452454\B9=1.094892
54\B10=1.53847097\B11=1.09153936\B12=1.09471545\B13=1.35731842\A1=120.
07716818\A2=103.94734772\A3=79.68323225\A4=102.17913213\A5=119.8822665
4\A6=118.14023902\A7=112.97332062\A8=111.71018244\A9=106.28196318\A10=
111.37416487\A11=110.26534955\A12=123.88881795\D1=47.07877692\D2=-66.8
7510303\D3=174.61456167\D4=-104.61867573\D5=52.20971037\D6=-190.509870
15\D7=46.61461603\D8=-71.41012911\D9=-176.13274186\D10=-54.99585418\D1
1=217.83892241\B2=2.14638813\\Version=AM64L-G09RevC.01\State=2-A\HF=-3
43.1279962\MP2=-344.2025684\PUHF=-343.1464056\PMP2-0=-344.2184991\S2=1
.001262\S2-1=0.931499\S2A=0.763168\RMSD=4.830e-09\RMSF=1.209e-05\Dipol
e=0.0955499,-0.023012,-1.3980075\PG=C01 [X(C5H7O2)]\\@

MP2/6-311++G(d,p)

1\1\GINC-GOMBERG10\FTS\UMP2-FC\6-311++G(d,p)\C5H7O2(2)\CARLHS\07-Jan-2
014\1\\#mp2=direct/6-311++G** opt=(grad,ts,readfc,noeigentest,nofreeze
) geom=checkpoint guess=read\\Oxyacyl radical endo transition state\\0
,2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1
,A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,
8,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,
A11,6,D10,0\O,1,B13,2,A12,3,D11,0\\B1=1.19197689\B3=1.08535091\B4=1.08
796764\B5=1.35122363\B6=1.08709633\B7=1.49409404\B8=1.09462757\B9=1.09
506247\B10=1.53770821\B11=1.09164223\B12=1.09468426\B13=1.35560459\A1=
119.92248199\A2=103.97667654\A3=79.76388368\A4=101.51665445\A5=119.895
05533\A6=118.22745455\A7=112.95943226\A8=111.67732528\A9=106.45975603\
A10=111.3527511\A11=110.59329769\A12=123.8956738\D1=47.17207026\D2=-66
.90380297\D3=174.34141398\D4=-104.89421635\D5=52.6906035\D6=-191.46635
23\D7=45.78890838\D8=-72.49277578\D9=-176.75901172\D10=-55.34635263\D1
1=216.73873684\B2=2.15091601\\Version=AM64L-G09RevC.01\State=2-A\HF=-3
43.1342622\MP2=-344.2170532\PUHF=-343.152307\PMP2-0=-344.2326486\S2=0.
995964\S2-1=0.927163\S2A=0.762607\RMSD=5.541e-09\RMSF=4.271e-05\Dipole
=0.1339439,-0.0341527,-1.5413256\PG=C01 [X(C5H7O2)]\\@

MP2/cc-pVDZ

1\1\GINC-GOMBERG03\FTS\UMP2-FC\CC-pVDZ\C5H7O2(2)\CARLHS\07-Jan-2014\1\
\#mp2=direct/cc-pVDZ opt=(grad,ts,readfc,noeigentest,nofreeze) geom=ch
eckpoint guess=read\\Oxyacyl radical endo transition state\\0,2\C\O,1,
B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,
0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8
,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10
,0\O,1,B13,2,A12,3,D11,0\\B1=1.1960992\B3=1.09439535\B4=1.09646335\B5=
1.35853203\B6=1.09620882\B7=1.49860384\B8=1.10306569\B9=1.10397295\B10
=1.54056446\B11=1.10073729\B12=1.10413912\B13=1.36462302\A1=120.683932
75\A2=104.05265525\A3=79.57041189\A4=102.04925266\A5=119.80758468\A6=1
18.13469975\A7=112.97453856\A8=111.87207\A9=106.4151651\A10=111.312951
2\A11=110.2274855\A12=123.63330518\D1=46.43792043\D2=-67.42944182\D3=1
74.01652773\D4=-104.72868248\D5=52.25103639\D6=-190.33171602\D7=47.045

20446\D8=-71.2696521\D9=-176.14331239\D10=-55.59572366\D11=217.1949557
6\B2=2.15565857\\Version=AM64L-G09RevC.01\State=2-A\HF=-343.0678167\MP
2=-344.0819774\PUHF=-343.0863966\PMP2-0=-344.0980898\S2=1.007235\S2-1=
0.936733\S2A=0.76385\RMSD=6.669e-09\RMSF=2.075e-05\Dipole=0.0858419,-0
.0186944,-1.3458385\PG=C01 [X(C5H7O2)]\\@

MP2/aug-cc-pVDZ

1\1\GINC-GOMBERG03\FTS\UMP2-FC\Aug-CC-pVDZ\C5H7O2(2)\CARLHS\07-Jan-201
4\1\\#mp2=direct/aug-cc-pVDZ opt=(grad,ts,readfc,noeigentest,nofreeze)
geom=checkpoint guess=read\\Oxyacyl radical endo transition state\\0,
2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,
A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8
,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A
11,6,D10,0\O,1,B13,2,A12,3,D11,0\\B1=1.20306979\B3=1.09238535\B4=1.095
23755\B5=1.35824406\B6=1.0943429\B7=1.49917658\B8=1.10188297\B9=1.1020
8221\B10=1.5422232\B11=1.09906579\B12=1.1019154\B13=1.36738502\A1=119.
62912334\A2=103.48828395\A3=79.47739344\A4=101.52641296\A5=119.8446375
2\A6=118.40418059\A7=112.89402883\A8=112.00593874\A9=106.10320618\A10=
111.56739614\A11=110.73068265\A12=123.31839198\D1=48.18969927\D2=-66.0
3865062\D3=175.27620259\D4=-104.73283195\D5=53.36965174\D6=-190.965471
83\D7=45.94827745\D8=-72.49373707\D9=-177.12796667\D10=-55.40358947\D1
1=218.84628293\B2=2.14810213\\Version=AM64L-G09RevC.01\State=2-A\HF=-3
43.0876082\MP2=-344.1534569\PUHF=-343.1057289\PMP2-0=-344.1691469\S2=1
.000215\S2-1=0.930951\S2A=0.763441\RMSD=8.515e-09\RMSF=2.654e-05\Dipol
e=0.1420986,-0.0080998,-1.5681759\PG=C01 [X(C5H7O2)]\\@

ROMP2/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.227708

QCISD/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.275843

CCSD(T)/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -344.318827

ROMP2/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.229562

QCISD/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.276933

CCSD(T)/6-311++G(d,p)//MP2/6-311++G(d,p) = -344.320616

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.163327

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.216127

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -344.257411

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.166370

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.218242

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -344.260521

Transition State 3 X=CH2 endo Boat

HF/6-31G(d)

1\1\GINC-GOMBERG03\FTS\UHF\6-31G(d)\C6H9O1(2)\AHANCOCK\23-Apr-2013\1\\
#P Geom=AllCheck Guess=Read HF/6-31G* opt=(grad,nofreeze,ts,noeigentes
t,readfc)\\9-1-A Benchmark\\0,2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,
0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6
,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11
,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B1
4,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=1.17236009\B3=1.07529542\B4
=1.07548652\B5=1.38823874\B6=1.07632101\B7=1.5110019\B8=1.08648236\B9=
1.08862728\B10=1.53971723\B11=1.0854309\B12=1.08588498\B13=1.52423426\
B14=1.08652686\B15=1.08733267\A1=122.52454763\A2=102.08017356\A3=93.58
595069\A4=95.19947004\A5=118.76911095\A6=121.17792402\A7=108.94747704\
A8=111.49717508\A9=111.60717603\A10=109.41658473\A11=109.99610947\A12=
126.7947282\A13=106.17873177\A14=107.45047705\D1=-4.66935893\D2=-121.2
3010116\D3=117.62639013\D4=-97.3154519\D5=66.68009104\D6=-152.01723727
\D7=91.16544641\D8=-31.43924417\D9=-168.21801031\D10=75.55678972\D11=1
54.54615529\D12=63.03399039\D13=-50.86456488\B2=2.1684778\\Version=AM6
4L-G09RevC.01\State=2-A\HF=-307.220567\S2=1.024623\S2-1=0.\S2A=0.76374
7\RMSD=9.582e-09\RMSF=2.970e-05\Dipole=-0.2486905,-0.1983631,-1.126984
1\Quadrupole=2.5166321,2.5871004,-5.1037326,0.0028084,1.2479691,-1.390
9389\PG=C01 [X(C6H9O1)]\\@

HF/6-311G(d,p)

1\1\GINC-GOMBERG16\FTS\UHF\6-311G(d,p)\C6H9O1(2)\AHANCOCK\23-Apr-2013\
1\\#P Geom=AllCheck Guess=Read HF/6-311G** opt=(grad,nofreeze,ts,noeig
entest,readfc)\\9-1-A Benchmark\\0,2\C\O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,
2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7
,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0
\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,1,B13,2,A12,3,D11,0\H,
14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=1.16555705\B3=1.075694
28\B4=1.07582902\B5=1.38788743\B6=1.07679588\B7=1.51077214\B8=1.087035
41\B9=1.08891173\B10=1.5389166\B11=1.08564006\B12=1.0863243\B13=1.5237
2098\B14=1.08672158\B15=1.08790661\A1=122.22766743\A2=102.09664352\A3=
93.66233449\A4=95.27887845\A5=118.80833087\A6=121.10211366\A7=108.8791
8744\A8=111.46221414\A9=111.5726844\A10=109.44677075\A11=109.94728305\
A12=127.17632065\A13=105.93394984\A14=107.25495137\D1=-4.64893123\D2=-
121.35394275\D3=117.53835142\D4=-97.5648475\D5=66.69507533\D6=-151.579
27576\D7=91.58833632\D8=-30.99041666\D9=-168.33745498\D10=75.37940334\
D11=155.18130425\D12=63.48497907\D13=-50.40445001\B2=2.15800116\\Versi
on=AM64L-G09RevC.01\State=2-A\HF=-307.2956473\S2=1.015594\S2-1=0.\S2A=
0.763057\RMSD=9.130e-09\RMSF=1.624e-05\Dipole=-0.2821615,-0.1904902,-1
.1056215\Quadrupole=2.3492918,2.569707,-4.9189988,0.0076839,1.3344164,
-1.3765916\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/6-311G(d,p)

1\1\GINC-GOMBERG17\FTS\UBHandHLYP\6-311G(d,p)\C6H9O1(2)\AHANCOCK\27-Ma
r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/6-311G** freq=noraman
opt=(grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O,1,
B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,
0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8
,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10
,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0
\\B1=1.17450117\B3=1.07615009\B4=1.0759825\B5=1.35896579\B6=1.07764254

\B7=1.49979828\B8=1.08772395\B9=1.08993616\B10=1.53288627\B11=1.085885
07\B12=1.08650512\B13=1.51879254\B14=1.08797008\B15=1.08954436\A1=119.
37005539\A2=101.41425571\A3=92.70060661\A4=92.80088453\A5=118.90842976
\A6=121.65537569\A7=109.07197527\A8=111.87419987\A9=110.74743186\A10=1
09.85977245\A11=109.97392062\A12=127.0569703\A13=105.23182203\A14=107.
8473571\D1=-15.56438681\D2=-132.09107747\D3=106.26602829\D4=-97.005493
24\D5=70.01437092\D6=-152.49117197\D7=90.50012866\D8=-32.12943301\D9=-
169.35209089\D10=74.06402231\D11=146.49831695\D12=76.36193164\D13=-37.
40986398\B2=2.14755374\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.070
2164\S2=0.811035\S2-1=0.\S2A=0.750682\RMSD=5.207e-09\RMSF=1.750e-05\Di
pole=-0.2240879,-0.277886,-1.0342367\Quadrupole=1.9859366,1.9243047,-3
.9102413,0.1390166,1.5804449,-1.580312\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/6-311++G(d,p)

1\1\GINC-GOMBERG17\FTS\UBHandHLYP\6-311++G(d,p)\C6H9O1(2)\AHANCOCK\28-
Mar-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/6-311++G** freq=nora
man opt=(grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\
O,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2
,D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,
6,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6
,D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D
13,0\\B1=1.17591732\B3=1.07622645\B4=1.07594771\B5=1.35951969\B6=1.077
73893\B7=1.49963023\B8=1.08775366\B9=1.0899035\B10=1.53274535\B11=1.08
594491\B12=1.08657329\B13=1.51650792\B14=1.08809523\B15=1.08978378\A1=
119.10690357\A2=101.58485921\A3=92.61727335\A4=92.63308247\A5=118.8750
8727\A6=121.70846012\A7=109.05290173\A8=111.80688566\A9=110.76485092\A
10=109.83759146\A11=110.03125589\A12=127.25262858\A13=105.1839374\A14=
107.94275318\D1=-15.54089682\D2=-132.10322259\D3=106.25190089\D4=-97.1
5219054\D5=69.97680688\D6=-152.42979949\D7=90.60834357\D8=-31.99512146
\D9=-169.30624175\D10=74.10737765\D11=146.73806331\D12=76.63833728\D13
=-37.16770171\B2=2.14645655\\Version=AM64L-G09RevC.01\State=2-A\HF=-30
9.0755048\S2=0.809592\S2-1=0.\S2A=0.750665\RMSD=4.361e-09\RMSF=2.214e-
05\Dipole=-0.2191633,-0.3078034,-1.1354314\Quadrupole=2.1536319,2.1030
717,-4.2567037,0.2006083,1.7934807,-1.6708238\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-GOMBERG12\FTS\UBHandHLYP\CC-pVDZ\C6H9O1(2)\AHANCOCK\28-Mar-20
13\1\\#P Geom=AllCheck Guess=Read BHandHLYP/cc-pVDZ freq=noraman opt=(
grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O,1,B1\C,
1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6
,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7
,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,
1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=
1.17955284\B3=1.08432183\B4=1.08374437\B5=1.36297078\B6=1.08599774\B7=
1.50106359\B8=1.09570496\B9=1.09799898\B10=1.53175191\B11=1.0938257\B1
2=1.09471887\B13=1.51967723\B14=1.09592383\B15=1.09757953\A1=119.66499
573\A2=101.79187338\A3=91.887056\A4=92.88507198\A5=118.80845473\A6=121
.75126376\A7=109.01014642\A8=111.9456451\A9=110.87327781\A10=109.88425
899\A11=110.07516224\A12=126.98990326\A13=105.12472731\A14=107.8487598
3\D1=-16.08028695\D2=-132.60396631\D3=105.82937766\D4=-97.58097971\D5=
69.31644435\D6=-151.32589363\D7=91.88770105\D8=-30.92326524\D9=-170.21
239979\D10=73.39211467\D11=146.37393614\D12=76.89028026\D13=-36.597355
1\B2=2.1579044\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.0082383\S2=
0.811891\S2-1=0.\S2A=0.750695\RMSD=9.422e-09\RMSF=2.090e-05\Dipole=-0.
2223111,-0.2679988,-0.9963386\Quadrupole=1.940175,1.7875714,-3.7277464

,0.1131853,1.4644841,-1.5260819\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-GOMBERG17\FTS\UBHandHLYP\Aug-CC-pVDZ\C6H9O1(2)\AHANCOCK\03-Ap
r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/aug-cc-pVDZ freq=noram
an opt=(grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O
,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,
D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6
,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,
D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D1
3,0\\B1=1.18187442\B3=1.08167774\B4=1.08128017\B5=1.36284432\B6=1.0834
0609\B7=1.50084837\B8=1.09262083\B9=1.09486396\B10=1.53287416\B11=1.09
098017\B12=1.09118562\B13=1.51717276\B14=1.09287948\B15=1.09465928\A1=
118.67055711\A2=101.47750389\A3=92.51351547\A4=92.11155107\A5=118.7594
6122\A6=121.83461124\A7=108.99180126\A8=111.89065651\A9=110.65506444\A
10=109.80808523\A11=110.10315172\A12=127.09282892\A13=105.08525096\A14
=107.96122031\D1=-16.30479716\D2=-133.00697968\D3=105.30474371\D4=-96.
96986716\D5=70.39748293\D6=-152.83222506\D7=90.08779923\D8=-32.5372690
2\D9=-169.07029096\D10=74.23701467\D11=145.71221058\D12=77.86102089\D1
3=-36.06971151\B2=2.15043193\\Version=AM64L-G09RevC.01\State=2-A\HF=-3
09.0282667\S2=0.808665\S2-1=0.\S2A=0.750679\RMSD=9.065e-09\RMSF=2.016e
-05\Dipole=-0.1869788,-0.319891,-1.1329681\Quadrupole=2.1089525,2.0675
264,-4.1764789,0.2074428,1.8082641,-1.7044322\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-GOMBERG18\FTS\UBHandHLYP\CC-pVTZ\C6H9O1(2)\AHANCOCK\03-Apr-20
13\1\\#P Geom=AllCheck Guess=Read BHandHLYP/cc-pVTZ freq=noraman opt=(
grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O,1,B1\C,
1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6
,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7
,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,
1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=
1.17430981\B3=1.07369464\B4=1.07336336\B5=1.35563461\B6=1.07518236\B7=
1.49623784\B8=1.08535675\B9=1.08760994\B10=1.52928991\B11=1.08351479\B
12=1.0840374\B13=1.5137394\B14=1.08573648\B15=1.08729112\A1=119.120232
67\A2=101.57529189\A3=92.6722462\A4=92.60374888\A5=118.86193392\A6=121
.76400664\A7=109.04631126\A8=111.90958385\A9=110.75433128\A10=109.8524
6667\A11=110.01111604\A12=127.21076615\A13=105.19941665\A14=107.888195
26\D1=-15.95031177\D2=-132.48281158\D3=105.84176953\D4=-97.05693417\D5
=70.00108374\D6=-152.15793891\D7=90.89491091\D8=-31.79182982\D9=-169.4
2619942\D10=74.00123172\D11=146.58278465\D12=77.03247676\D13=-36.69252
704\B2=2.13915202\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.101743\S
2=0.808987\S2-1=0.\S2A=0.750684\RMSD=8.703e-09\RMSF=2.275e-05\Dipole=-
0.2101593,-0.2885914,-1.0646901\Quadrupole=2.0041199,1.9439657,-3.9480
856,0.1659487,1.6248025,-1.6071473\PG=C01 [X(C6H9O1)]\\@

BHandHLYP/aug-cc-pVTZ

1\1\GINC-GOMBERG18\FTS\UBHandHLYP\Aug-CC-pVTZ\C6H9O1(2)\AHANCOCK\04-Ap
r-2013\1\\#P Geom=AllCheck Guess=Read BHandHLYP/aug-cc-pVTZ freq=noram
an opt=(grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O
,1,B1\C,1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,
D3,0\H,6,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6
,A8,3,D7,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,
D10,0\C,1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D1
3,0\\B1=1.17445291\B3=1.07362917\B4=1.07329086\B5=1.35563712\B6=1.0751

46\B7=1.49609156\B8=1.08522073\B9=1.08743937\B10=1.52924086\B11=1.0833
9315\B12=1.08390526\B13=1.51319438\B14=1.08561191\B15=1.08727926\A1=11
8.93499347\A2=101.6179779\A3=92.70890434\A4=92.48758315\A5=118.8502669
9\A6=121.77156821\A7=109.04475657\A8=111.87617999\A9=110.74863616\A10=
109.85167163\A11=110.02930691\A12=127.32862236\A13=105.19377512\A14=10
7.89129656\D1=-15.97811806\D2=-132.54698121\D3=105.79229881\D4=-97.003
05592\D5=70.08800289\D6=-152.26609586\D7=90.7771343\D8=-31.87657627\D9
=-169.35169293\D10=74.05009229\D11=146.62749399\D12=77.19845616\D13=-3
6.58735033\B2=2.13838325\\Version=AM64L-G09RevC.01\State=2-A\HF=-309.1
053012\S2=0.808073\S2-1=0.\S2A=0.750675\RMSD=3.832e-09\RMSF=2.279e-05\
Dipole=-0.2005787,-0.3023732,-1.1158762\Quadrupole=2.0729973,2.0524859
,-4.1254831,0.1930804,1.7595011,-1.6403957\PG=C01 [X(C6H9O1)]\\@

MP2/6-311G(d,p)

1\1\GINC-GOMBERG08\FTS\UMP2-FC\6-311G(d,p)\C6H9O1(2)\AHANCOCK\02-Apr-2
013\1\\#P Geom=AllCheck Guess=Read MP2/6-311G** freq=noraman opt=(grad
,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O,1,B1\C,1,B2
,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,B6,
3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,0\C
,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,1,B1
3,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=1.19
564374\B3=1.0852613\B4=1.0846247\B5=1.34747982\B6=1.08687382\B7=1.5055
0697\B8=1.09623152\B9=1.09781465\B10=1.53993715\B11=1.09490877\B12=1.0
9462621\B13=1.5337609\B14=1.09671983\B15=1.0987062\A1=118.05792158\A2=
99.54373639\A3=94.22221727\A4=90.20437453\A5=118.9222258\A6=121.507862
88\A7=109.27234464\A8=112.17349309\A9=109.23558733\A10=110.23196561\A1
1=109.93634042\A12=126.35497734\A13=105.17740393\A14=108.37311505\D1=-
20.80903328\D2=-137.83700646\D3=100.31053647\D4=-93.96171579\D5=74.851
64684\D6=-154.78699767\D7=86.98647963\D8=-35.39956281\D9=-169.1801997\
D10=73.34888598\D11=143.26686429\D12=81.56482398\D13=-33.13985186\B2=2
.10998904\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.2905803\MP2=-308
.329453\PUHF=-307.3064275\PMP2-0=-308.3430599\S2=0.962656\S2-1=0.90096
5\S2A=0.759327\RMSD=7.487e-09\RMSF=3.415e-05\Dipole=-0.1391551,-0.3019
058,-0.9069505\PG=C01 [X(C6H9O1)]\\@

MP2/6-311++G(d,p)

1\1\GINC-GOMBERG10\FTS\UMP2-FC\6-311++G(d,p)\C6H9O1(2)\AHANCOCK\21-Apr
-2013\1\\#P Geom=AllCheck Guess=Read MP2/6-311++G** freq=noraman opt=(
grad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O,1,B1\C,
1,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6
,B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7
,0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,
1,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=
1.19855567\B3=1.08535354\B4=1.08475516\B5=1.34828705\B6=1.08712676\B7=
1.50541965\B8=1.09621098\B9=1.09777314\B10=1.54003935\B11=1.0948832\B1
2=1.09486007\B13=1.53049703\B14=1.09684964\B15=1.0991894\A1=117.602420
88\A2=99.7450568\A3=94.30178194\A4=89.7144006\A5=118.85835314\A6=121.5
9965343\A7=109.24250958\A8=112.09839112\A9=109.21707474\A10=110.206574
86\A11=110.074666\A12=126.58533511\A13=105.14105572\A14=108.52154233\D
1=-21.05413932\D2=-138.14760246\D3=100.02084377\D4=-93.85109113\D5=75.
05803485\D6=-154.97067747\D7=86.87883107\D8=-35.4682408\D9=-169.001741
6\D10=73.52999675\D11=143.46316063\D12=82.16821462\D13=-32.59701371\B2
=2.10768294\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.295057\MP2=-30
8.3397738\PUHF=-307.3106011\PMP2-0=-308.3531068\S2=0.9587\S2-1=0.89780

7\S2A=0.758981\RMSD=3.649e-09\RMSF=3.912e-05\Dipole=-0.1285591,-0.3522
984,-1.0316028\PG=C01 [X(C6H9O1)]\\@

MP2/cc-pVDZ

1\1\GINC-GOMBERG13\FTS\UMP2-FC\CC-pVDZ\C6H9O1(2)\AHANCOCK\02-Apr-2013\
1\\#P Geom=AllCheck Guess=Read MP2/cc-pVDZ freq=noraman opt=(grad,nofr
eeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O,1,B1\C,1,B2,2,A1
\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,B6,3,A5,
1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,0\C,8,B1
0,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,1,B13,2,A
12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=1.2015265
7\B3=1.0940573\B4=1.0930003\B5=1.35587375\B6=1.09588526\B7=1.5095524\B
8=1.10504196\B9=1.10671543\B10=1.54148968\B11=1.10368842\B12=1.1040480
1\B13=1.53840791\B14=1.10557912\B15=1.10765828\A1=118.95463889\A2=100.
2145221\A3=92.92873087\A4=90.98139054\A5=118.84954604\A6=121.54096523\
A7=109.18945985\A8=112.26383391\A9=109.54834053\A10=110.2037971\A11=11
0.16578111\A12=126.40787082\A13=105.06104509\A14=108.35625213\D1=-20.3
7186844\D2=-137.21267021\D3=100.98799489\D4=-95.04704421\D5=73.3896593
\D6=-152.65306244\D7=89.59893482\D8=-33.17118654\D9=-170.19562461\D10=
72.795801\D11=144.21111431\D12=80.64408672\D13=-33.52060344\B2=2.12020
745\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.2391331\MP2=-308.22137
67\PUHF=-307.2552931\PMP2-0=-308.2352821\S2=0.969812\S2-1=0.906827\S2A
=0.759971\RMSD=4.856e-09\RMSF=3.215e-05\Dipole=-0.1614866,-0.2809952,-
0.8711747\PG=C01 [X(C6H9O1)]\\@

MP2/aug-cc-pVDZ

1\1\GINC-GOMBERG13\FTS\UMP2-FC\Aug-CC-pVDZ\C6H9O1(2)\AHANCOCK\03-Apr-2
013\1\\#P Geom=AllCheck Guess=Read MP2/aug-cc-pVDZ freq=noraman opt=(g
rad,nofreeze,ts,noeigentest,readfc)\\9-1-A Benchmark\\0,2\C\O,1,B1\C,1
,B2,2,A1\H,3,B3,1,A2,2,D1,0\H,3,B4,1,A3,2,D2,0\C,3,B5,1,A4,2,D3,0\H,6,
B6,3,A5,1,D4,0\C,6,B7,3,A6,1,D5,0\H,8,B8,6,A7,3,D6,0\H,8,B9,6,A8,3,D7,
0\C,8,B10,6,A9,3,D8,0\H,11,B11,8,A10,6,D9,0\H,11,B12,8,A11,6,D10,0\C,1
,B13,2,A12,3,D11,0\H,14,B14,1,A13,2,D12,0\H,14,B15,1,A14,2,D13,0\\B1=1
.21029113\B3=1.09232973\B4=1.09191158\B5=1.35530779\B6=1.0941259\B7=1.
51036281\B8=1.10328928\B9=1.10475914\B10=1.54456311\B11=1.10220539\B12
=1.10198424\B13=1.53515643\B14=1.10397414\B15=1.10651816\A1=117.105698
35\A2=99.61632836\A3=94.09948734\A4=88.97818114\A5=118.72844414\A6=121
.74474445\A7=109.22308907\A8=112.08051193\A9=109.05924666\A10=110.2397
7252\A11=110.29818748\A12=126.4358604\A13=105.13053878\A14=108.3989833
6\D1=-22.26382278\D2=-139.48187189\D3=98.67166517\D4=-93.51312088\D5=7
5.52736565\D6=-154.78262491\D7=87.14782743\D8=-35.42635045\D9=-169.250
67394\D10=73.25568209\D11=142.70125617\D12=83.46947458\D13=-31.2557597
8\B2=2.10924225\\Version=AM64L-G09RevC.01\State=2-A\HF=-307.2541151\MP
2=-308.2810394\PUHF=-307.2695779\PMP2-0=-308.2943107\S2=0.95901\S2-1=0
.898213\S2A=0.75924\RMSD=8.660e-09\RMSF=8.330e-06\Dipole=-0.0867147,-0
.376875,-1.0654366\PG=C01 [X(C6H9O1)]\\@

ROMP2/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.350060

QCISD/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.409500

CCSD(T)/6-311++G(d,p)//BHandHLYP/6-311++G(d,p) = -308.452145

ROMP2/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.350060

QCISD/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.409573

CCSD(T)/6-311++G(d,p)//MP2/6-311++G(d,p) = -308.452145

ROMP2/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.290645

QCISD/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.354388

CCSD(T)/aug-cc-pVDZ//BHandHLYP/aug-cc-pVDZ = -308.395510

ROMP2/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.563892

QCISD/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.355748

CCSD(T)/aug-cc-pVDZ//MP2/aug-cc-pVDZ = -308.397735