Electronic Supplementary Information (ESI)

Multi-Component Orbital Interactions During Oxyacyl Radical Addition Reactions Involving Imines and Electron-Rich Olefins†

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UHF/6-311G** calculated energy barriers $\Delta E_1^{\ddagger} - \Delta E_4^{\ddagger}$ for reactions depicted in Schemes 4 and 5.

Gaussian Archive entries for optimised transition structures (**7** – **10**) (11 pages).

Table UHF/6-311G** calculated energy barriers[a] for the forward ($\Delta E_1^{\ddagger}$, $\Delta E_3^{\ddagger}$) and reverse ($\Delta E_2^{\ddagger}$, $\Delta E_4^{\ddagger}$) reactions depicted in Schemes 4 and 5, and imaginary frequencies (ν)[b] of transition states **7** – **10**.

	7 or **9**					**8** or **10**				
Scheme	$\Delta E_1^{\ddagger}$	$\Delta E_1^{\ddagger}$ +ZPE	$\Delta E_2^{\ddagger}$	$\Delta E_2^{\ddagger}$ +ZPE	ν	$\Delta E_3^{\ddagger}$	$\Delta E_3^{\ddagger}$ +ZPE	$\Delta E_4^{\ddagger}$	$\Delta E_4^{\ddagger}$ +ZPE	ν
Scheme 4	33.6	35.0	163.8	154.8	409i	47.3	48.3	216.0	205.8	524i
Scheme 5 (R = H)	32.8	32.7	155.6	146.4	381i	-	-	-	-	-
Scheme 5 (R = NH_2)	29.3	30.8	159.8	148.3	427i	34.6	34.9	143.1	133.8	465i
Scheme 5 (R = CF_3)	26.7	26.1	160.9	152.0	365i	35.8	34.9	147.9	140.3	339i

[a] Energies in kJ mol^{-1}. [b] Frequencies in cm^{-1}.

Gaussian Archive Entries for Transition States 7 – 10

Transition State 7

UHF/6-311G**

1\1\GINC-DUAL1\FTS\UHF\6-311G(d,p)\C3H6N1O2(2)\MATSU\12-Sep-2007\1\\#HF
/6-311G** SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE=100) NOSYMM FREQ=NORAMA
N GEOM=CHECK GUESS=READ\\TS oxyacyl radical to imine carbon\\0,2\C\O,1,
r2\O,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,d6,0
\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9,1,a
9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\\r2=1.16659998\r3=
1.29966685\a3=129.79965723\r4=2.20353821\a4=121.72478558\d4=188.1800049
3\r5=1.31255111\a5=102.27872358\d5=71.24994228\r6=1.4297556\a6=116.9486
7633\d6=-1.20214967\r7=1.08102565\a7=109.92218874\d7=-60.41455741\r8=1.
07796318\a8=105.67726744\d8=180.19967022\r81=1.08114446\a81=110.0535047
1\d81=60.70204645\r9=1.07741905\a9=92.80184254\d9=190.32819769\r10=1.08
134561\a10=91.9606694\d10=-52.75498834\r11=1.00657717\a11=109.96940884\
d11=-87.19923161\\Version=x86-Linux-G03RevB.05\HF=-321.2606973\S2=1.001
182\S2-1=0.\S2A=0.759374\RMSD=8.814e-09\RMSF=1.098e-06\Dipole=0.6002624
,-0.6257404,-0.1412053\Polar=55.649393,-6.7881908,40.1918977,2.1823151
,-0.6469846,43.4753999\HyperPolar=60.3329195,-7.5680742,-34.5529333,27.
4650395,14.6060141,-9.4844588,23.2035127,5.6413428,-14.7762817,-38.3794
345\PG=C01 [X(C3H6N1O2)]\\@

BHnadHLYP/6-311G**

1\1\GINC-DUAL1\FTS\UBHandHLYP\6-311G(d,p)\C3H6N1O2(2)\MATSU\12-Sep-2007
\1\\#BHANDHLYP/6-311G** SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE=100) NOSY
MM GEOM=CHECK GUESS=READ\\TS oxyacyl radical to imine carbon\\0,2\C\O,1
,r2\O,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,d6,
0\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9,1,
a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\\r2=1.17440029\r3
=1.30236458\a3=130.1040807\r4=2.2100405\a4=122.14184133\d4=194.49731866
\r5=1.28921781\a5=102.71333712\d5=75.03219934\r6=1.43925219\a6=116.1179
2763\d6=-1.30117873\r7=1.08234081\a7=109.67999154\d7=-60.78603434\r8=1.
0788128\a8=105.56525628\d8=179.79049447\r81=1.08237937\a81=109.90266417
\d81=60.17020086\r9=1.08118974\a9=90.2679565\d9=193.80557723\r10=1.0850
9688\a10=90.8459954\d10=-49.93439385\r11=1.01253055\a11=110.04217518\d1
1=-89.06512553\\Version=x86-Linux-G03RevB.05\HF=-322.9213248\S2=0.81201
8\S2-1=0.\S2A=0.750598\RMSD=4.843e-09\RMSF=6.891e-06\Dipole=0.6548142,-
0.6198406,0.0019183\Polar=60.9588807,-9.7441096,45.0032412,4.2120159,-2
.6618687,45.9324853\PG=C01 [X(C3H6N1O2)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-DUAL1\FTS\UBHandHLYP\CC-pVDZ\C3H6N1O2(2)\MATSU\12-Sep-2007\1\\
#BHANDHLYP/CC-PVDZ SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE=100) NOSYMM GE
OM=CHECK GUESS=READ\\TS oxyacyl radical to imine carbon\\0,2\C\O,1,r2\O
,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,d6,0\H,6
,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9,1,a9,2,
d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\\r2=1.17956985\r3=1.30
776066\a3=129.69882332\r4=2.22015404\a4=123.02672419\d4=194.58928587\r5
=1.29215895\a5=102.73560479\d5=77.68240338\r6=1.43740968\a6=115.6739925
1\d6=-0.9922864\r7=1.09082004\a7=109.84871995\d7=-59.8869514\r8=1.08734
74\a8=105.65399835\d8=180.59905013\r81=1.09092599\a81=110.04395349\d81=
60.95631508\r9=1.09007106\a9=89.8755497\d9=196.30930574\r10=1.09360037\
a10=90.6308205\d10=-47.63006098\r11=1.0197748\a11=109.51682901\d11=-89.
27365984\\Version=x86-Linux-G03RevB.05\HF=-322.8524704\S2=0.813041\S2-1
=0.\S2A=0.750609\RMSD=7.404e-09\RMSF=6.512e-06\Dipole=0.603942,-0.55232
09,0.016232\Polar=59.4410398,-9.4167436,43.7616501,4.2931189,-2.7549778
,44.8902596\PG=C01 [X(C3H6N1O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-DUAL1\FTS\UBHandHLYP\Aug-CC-pVDZ\C3H6N1O2(2)\MATSU\12-Sep-2007
\1\\#BHANDHLYP/AUG-CC-PVDZ SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE=100) N

OSYMM GEOM=CHECK GUESS=READ\\TS oxyacyl radical to carbon imine\\0,2\C\
O,1,r2\O,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,
d6,0\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9
,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\\r2=1.18106767
\r3=1.3051071\a3=130.23548843\r4=2.22491606\a4=121.48365499\d4=194.0585
208\r5=1.29218461\a5=102.53413575\d5=81.22466942\r6=1.44306111\a6=116.0
2677418\d6=-1.42062365\r7=1.08780584\a7=109.50209038\d7=-60.07633199\r8
=1.08470901\a8=105.38865827\d8=180.51006697\r81=1.08787609\a81=109.7512
2715\d81=60.90289508\r9=1.08658524\a9=90.47807796\d9=200.0118801\r10=1.
08990336\a10=90.26293988\d10=-43.28598476\r11=1.01509126\a11=110.439607
82\d11=-88.84656891\\Version=x86-Linux-G03RevB.05\HF=-322.8803003\S2=0.
809008\S2-1=0.\S2A=0.750591\RMSD=7.743e-09\RMSF=7.065e-06\Dipole=0.6363
356,-0.6039648,0.0058062\Polar=70.9053967,-10.0345996,53.5017001,5.9590
54,-4.483869,54.5693123\PG=C01 [X(C3H6N1O2)]\\@

Transition State 8

UHF/6-311G**

1\1\GINC-DUAL1\FTS\UHF\6-311G(d,p)\C3H6N1O2(2)\MATSU\12-Sep-2007\1\\#HF
/6-311G** SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE=100) NOSYMM FREQ=NORAMA
N GEOM=CHECK GUESS=READ\\TS oxyacyl radical to imine nitrogen\\0,2\C\O,
1,r2\O,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,d6
,0\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9,1
,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\\r2=1.16912655\r
3=1.3057523\a3=129.0915629\r4=1.98291729\a4=119.51577889\d4=149.6485652
8\r5=1.31077833\a5=114.91106321\d5=31.9281656\r6=1.42559592\a6=116.7595
9142\d6=1.97341472\r7=1.08137359\a7=110.30374051\d7=-60.87518379\r8=1.0
7857777\a8=105.82947075\d8=179.62601832\r81=1.08144696\a81=110.06620549
\d81=60.24111598\r9=1.00415404\a9=99.95563551\d9=151.97005195\r10=1.079
54764\a10=123.02535799\d10=108.33872804\r11=1.07572196\a11=118.40800541
\d11=-66.78508453\\Version=x86-Linux-G03RevB.05\HF=-321.2554879\S2=1.00
5633\S2-1=0.\S2A=0.759204\RMSD=8.914e-09\RMSF=1.046e-04\Dipole=0.088731
5,0.2688304,-0.6732094\Polar=70.0715981,8.1999993,33.9370041,1.3783567,
0.2356594,42.8519522\HyperPolar=-67.8168813,-27.8729236,-14.6298651,5.1
322066,-111.2783654,-18.7743867,11.4246419,-18.5689023,-0.5868073,-34.4
926121\PG=C01 [X(C3H6N1O2)]\\@

BHandHLYP/6-311G**

1\1\GINC-DUAL1\FTS\UBHandHLYP\6-311G(d,p)\C3H6N1O2(2)\MATSU\12-Sep-2007
\1\\#BHANDHLYP/6-311G** SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE=100) NOSY
MM GEOM=CHECK GUESS=READ \\TS oxyacyl radical to imine nitorgen\\0,2\C\
O,1,r2\O,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,
d6,0\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9
,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\\r2=1.18209329
\r3=1.31874402\a3=128.16919654\r4=1.97821899\a4=114.41627293\d4=135.270
00535\r5=1.27227692\a5=118.78982196\d5=29.09807163\r6=1.43117793\a6=115
.70758031\d6=3.71122255\r7=1.08285676\a7=110.4011876\d7=-59.72032085\r8
=1.07997097\a8=105.85114132\d8=180.64210127\r81=1.08362782\a81=110.0739
1526\d81=61.20853203\r9=1.00977298\a9=108.62015885\d9=161.82612291\r10=
1.08255072\a10=123.57294644\d10=130.34122735\r11=1.0796871\a11=118.2998
0419\d11=-46.97749449\\Version=x86-Linux-G03RevB.05\HF=-322.9221029\S2=
0.78682\S2-1=0.\S2A=0.750311\RMSD=3.406e-09\RMSF=9.073e-06\Dipole=-0.23
88103,-0.3347062,-0.6986165\Polar=78.3678786,21.2588846,42.9125605,0.73
6097,1.5162342,45.2280141\PG=C01 [X(C3H6N1O2)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-DUAL1\FTS\UBHandHLYP\CC-pVDZ\C3H6N1O2(2)\MATSU\12-Sep-2007\1\\
#BHANDHLYP/CC-PVDZ SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE=100) NOSYMM GE
OM=CHECK GUESS=READ\\TS oxyacyl radical to imine nitrogen\\0,2\C\O,1,r2
\O,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,d6,0\H
,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9,1,a9,
2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\\r2=1.187241\r3=1.32
385409\a3=127.84049162\r4=1.98251832\a4=114.43702307\d4=134.54746124\r5

=1.27606359\a5=118.51467981\d5=28.90936429\r6=1.42951427\a6=115.2360261
1\d6=3.15571548\r7=1.09145579\a7=110.5651209\d7=-60.47768583\r8=1.08857
275\a8=105.94743504\d8=179.86227443\r81=1.092102\a81=110.2573267\d81=60
.32826363\r9=1.01630828\a9=109.14875729\d9=161.25232252\r10=1.09120498\
a10=123.73555951\d10=130.68122592\r11=1.08870654\a11=118.10923478\d11=-
46.50468421\\Version=x86-Linux-G03RevB.05\HF=-322.8535225\S2=0.787179\S
2-1=0.\S2A=0.750318\RMSD=6.335e-09\RMSF=8.660e-06\Dipole=-0.2423476,-0.
3508204,-0.6910989\Polar=76.7353811,21.446687,41.3832362,0.8764508,1.29
69865,44.2361972\PG=C01 [X(C3H6N1O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-DUAL1\FTS\UBHandHLYP\Aug-CC-pVDZ\C3H6N1O2(2)\MATSU\12-Sep-2007
\1\\#BHANDHLYP/AUG-CC-PVDZ SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE=100) N
OSYMM GEOM=CHECK GUESS=READ\\TS oxyacyl radical to imine nitrogen\\0,2\
C\O,1,r2\O,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,
2,d6,0\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,
r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\\r2=1.188559
49\r3=1.32134699\a3=128.25289439\r4=1.99427626\a4=114.43337912\d4=135.6
858347\r5=1.27586466\a5=118.72392133\d5=28.16753251\r6=1.43512633\a6=11
5.77130674\d6=3.40077894\r7=1.08829512\a7=110.24928024\d7=-60.57047606\
r8=1.08576607\a8=105.684092\d8=179.81127481\r81=1.08883909\a81=109.8767
0729\d81=60.3681217\r9=1.01228984\a9=108.67610425\d9=160.50128641\r10=1
.08807802\a10=123.32069339\d10=130.16776257\r11=1.08542983\a11=118.4030
0871\d11=-47.50276405\\Version=x86-Linux-G03RevB.05\HF=-322.8796496\S2=
0.78546\S2-1=0.\S2A=0.750313\RMSD=8.082e-09\RMSF=5.279e-06\Dipole=-0.25
42618,-0.3488904,-0.7134207\Polar=88.1632046,20.5429833,52.9985617,1.41
22904,1.9659057,53.3597364\PG=C01 [X(C3H6N1O2)]\\@

Transition State 9 (R = H)

UHF/6-311G****

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET20\FTS\UHF\6-311G(d,p)\C4H7O2(2)\HI
ROSHI\12-Sep-2007\1\\#HF/6-311G** SCF=DIRECT OPT=(TS,EF,CALCFC,MAXCYCLE
=100) NOSYMM\\TS oxyacyl ethylene\\0,2\C\O,1,r2\O,1,r3,2,a3\C,1,r4,2,a4
,3,d4,0\C,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,d6,0\H,6,r7,3,a7,1,d7,0\H,6,r8
,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d
10,0\H,5,r11,4,a11,1,d11,0\H,5,r12,4,a12,1,d12,0\\r2=1.16844519\r3=1.30
514031\a3=128.7723018\r4=2.2465935\a4=122.06293481\d4=189.10241512\r5=1
.37623915\a5=106.65129591\d5=110.5828351\r6=1.42679332\a6=116.86191723\
d6=-0.07266379\r7=1.08142258\a7=110.13161459\d7=-60.3892784\r8=1.078436
79\a8=105.7957242\d8=180.15713646\r81=1.08143547\a81=110.20504156\d81=6
0.6786415\r9=1.07590975\a9=91.9012439\d9=232.50296146\r10=1.07500816\a1
0=89.72496929\d10=-11.13693108\r11=1.07572105\a11=121.16224437\d11=-86.
29007845\r12=1.07531011\a12=121.18798647\d12=88.01222978\\Version=x86-L
inux-G03RevB.04\HF=-305.2589945\S2=1.009651\S2-1=0.\S2A=0.761101\RMSD=5
.965e-09\RMSF=5.363e-07\Dipole=0.6290222,0.0322998,-0.5602366\Polar=56.
0737563,-5.8245791,45.6465912,5.3506393,-6.8720337,51.7521207\HyperPola
r=154.0796373,-38.3657463,10.0980261,10.8376652,77.4358046,-19.382302,5
.5278295,47.0916934,-1.5862352,-29.6059855\PG=C01 [X(C4H7O2)]\\@

BHandHLYP/6-311G****

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET16\FTS\UBHandHLYP\6-311G(d,p)\C4H7O
2(2)\HIROSHI\12-Sep-2007\1\\#BHANDHLYP/6-311G** SCF=DIRECT OPT=(TS,EF,C
ALCFC,MAXCYCLE=100) NOSYMM GEOM=CHECK GUESS=READ\\TS oxyacyl ethylene\\
0,2\C\O,1,r2\O,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\C,3,r6,1
,a6,2,d6,0\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\
H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,5,r12,
4,a12,1,d12,0\\r2=1.17692611\r3=1.31075069\a3=128.58717082\r4=2.2681433
\a4=122.47026218\d4=196.4363187\r5=1.34861861\a5=105.7509377\d5=103.108
02689\r6=1.43575411\a6=115.98588714\d6=0.28311739\r7=1.08278882\a7=109.
96312488\d7=-60.06835311\r8=1.07933509\a8=105.71612476\d8=180.36174511\
r81=1.08274417\a81=110.09198985\d81=60.7760269\r9=1.0764878\a9=90.07928
431\d9=224.91100709\r10=1.07585687\a10=88.41108053\d10=-18.63252272\r11
=1.07651648\a11=121.35821725\d11=-87.42044017\r12=1.07618705\a12=121.36

577121\d12=88.59238253\\Version=x86-Linux-G03RevB.04\HF=-306.8830587\S2
=0.813282\S2-1=0.\S2A=0.750643\RMSD=6.295e-09\RMSF=8.604e-06\Dipole=0.6
678103,0.0478058,-0.4632029\Polar=62.0396238,-9.5094397,52.5163744,7.77
51532,-10.4024327,55.0001256\PG=C01 [X(C4H7O2)]\\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET6\FTS\UBHandHLYP\CC-pVDZ\C4H7O2(2)\
HIROSHI\12-Sep-2007\1\\#BHANDHLYP/CC-PVDZ SCF=DIRECT OPT=(TS,EF,CALCFC,
MAXCYCLE=100) NOSYMM GEOM=CHECK GUESS=READ\\TS oxyacyl ethylene\\0,2\C\
O,1,r2\O,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\C,3,r6,1,a6,2,
d6,0\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,0\H,4,r9
,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,5,r12,4,a12,
1,d12,0\\r2=1.18176532\r3=1.31507787\a3=128.37344714\r4=2.28368502\a4=1
23.26252509\d4=195.73019337\r5=1.35248357\a5=106.0451724\d5=106.0991745
7\r6=1.43427222\a6=115.56271796\d6=0.41749528\r7=1.09125635\a7=110.1023
6364\d7=-59.53845336\r8=1.08784972\a8=105.80867869\d8=180.81521276\r81=
1.09128758\a81=110.2336541\d81=61.19372014\r9=1.08489218\a9=89.45613131
\d9=227.76884333\r10=1.08423381\a10=88.16036303\d10=-15.66601045\r11=1.
08526618\a11=121.31580776\d11=-87.62180786\r12=1.08490919\a12=121.32799
225\d12=88.29353961\\Version=x86-Linux-G03RevB.04\HF=-306.8164854\S2=0.
813929\S2-1=0.\S2A=0.750652\RMSD=7.055e-09\RMSF=6.793e-06\Dipole=0.6413
26,0.0354322,-0.4466128\Polar=60.1880095,-9.060578,50.9253007,7.3656383
,-10.5170182,54.8184807\PG=C01 [X(C4H7O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET2\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H7O2
(2)\HIROSHI\12-Sep-2007\1\\#BHANDHLYP/AUG-CC-PVDZ SCF=DIRECT OPT=(TS,EF
,CALCFC,MAXCYCLE=100) NOSYMM GEOM=CHECK GUESS=READ\\TS oxyacyl ethylene
\\0,2\C\O,1,r2\O,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\C,3,r6
,1,a6,2,d6,0\H,6,r7,3,a7,1,d7,0\H,6,r8,3,a8,1,d8,0\H,6,r81,3,a81,1,d81,
0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,5,r1
2,4,a12,1,d12,0\\r2=1.18375399\r3=1.3144888\a3=128.57029269\r4=2.2828\a
4=121.90516072\d4=197.73879649\r5=1.35304289\a5=104.78861208\d5=94.5041
3373\r6=1.43948944\a6=115.93044312\d6=0.28985981\r7=1.08821732\a7=109.7
9209034\d7=-59.93720324\r8=1.08522467\a8=105.56301795\d8=180.49496991\r
81=1.08812176\a81=109.93946003\d81=60.92291586\r9=1.0822339\a9=90.08939
336\d9=216.29097946\r10=1.08143699\a10=88.27771144\d10=-27.01184827\r11
=1.08225666\a11=121.32155743\d11=-87.4108061\r12=1.08217748\a12=121.353
05751\d12=89.13071364\\Version=x86-Linux-G03RevB.04\HF=-306.83923\S2=0.
810564\S2-1=0.\S2A=0.750625\RMSD=6.270e-09\RMSF=2.789e-06\Dipole=0.6337
798,0.0635452,-0.5247459\Polar=74.8660913,-11.3983085,61.5586046,9.5821
411,-9.9554107,62.1242209\PG=C01 [X(C4H7O2)]\\@

Transition State 9 (R = NH_2)

UHF/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET1\FTS\UHF\6-311G(d,p)\C4H8N1O2(2)\
SKYNE\11-Oct-2006\0\\#UHF/6-311G** OPT=(TS,CALCFC,NOEIGEN,MAXCYC=300)
SCF=QC FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radical addit
ion to the C1 (furthest to amine) end of the alkene bond, c\\0,2\N,-2.
6247258253,0.8830928442,0.0457332579\C,-1.2777956207,-1.0938706457,-0.
4342779315\C,0.6421264566,-0.420708394,0.4522201596\O,1.5683456762,-0.
3869390435,-0.4742477481\C,2.7035656795,0.4358311608,-0.2218790454\O,0
.6249904709,0.1631052274,1.4696876495\H,-2.4477146257,0.7149140152,1.0
129473333\H,-2.5692277246,1.856666344,-0.1581052919\H,3.2149405565,0.1
071485205,0.6726658245\H,2.3999522037,1.467575577,-0.1048602699\H,3.34
43031346,0.3270700686,-1.0829699838\H,-0.8666939643,-1.7334900361,-1.1
925628783\H,-1.5520528638,-1.5612173097,0.4952773433\C,-1.8886351077,0
.0752603737,-0.8145283122\H,-1.7726835633,0.4512784707,-1.8152533163\\
Version=x86-Linux-G03RevB.04\State=2-A\HF=-360.3076522\S2=0.9713\S2-1=
0.\S2A=0.758483\RMSD=0.000e+00\RMSF=3.054e-06\Dipole=0.50839,0.4600584
,-0.5474915\PG=C01 [X(C4H8N1O2)]\\@

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET19\FTS\UBHandHLYP\6-311G(d,p)\C4H8
N1O2(2)\SKYNE\20-Oct-2006\0\\#BHANDHLYP/6-311G** OPT=(TS,READFC,NOEIGE
N,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radica
l addition to the C1 (furthest to amine) end of the alkene bond, c\\0,
2\N,-2.36219559,-0.8256710992,0.4258484383\C,-1.3241705987,1.144791215
7,-0.4872648737\C,0.6426903788,0.085884379,-0.6716862588\O,1.555398463
4,0.683326531,0.0739523875\C,2.5339740645,-0.1712851187,0.6746849144\O
,0.5508645119,-1.0797665312,-0.8743139385\H,-2.0714547633,-1.334709182
8,-0.3877614462\H,-2.3527319979,-1.3862678285,1.2532246448\H,3.0884211
627,-0.7041897873,-0.0879275994\H,2.0542018178,-0.8864830147,1.3324110
889\H,3.1897089292,0.4786930268,1.234926678\H,-1.0076167924,2.15778611
06,-0.3257509074\H,-1.5190461295,0.8487307657,-1.5024434691\C,-1.83533
96943,0.4327556494,0.5439971686\H,-1.7991418007,0.8247808542,1.5468886
466\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-362.2298607\S2=0.79483
4\S2-1=0.\S2A=0.750395\RMSD=2.474e-09\RMSF=3.866e-06\Dipole=0.1369931,
-0.1468115,0.8999308\PG=C01 [X(C4H8N1O2)]\\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET11\FTS\UBHandHLYP\CC-pVDZ\C4H8N1O2
(2)\SKYNE\21-Oct-2006\0\\#BHANDHLYP/CC-PVDZ OPT=(TS,READFC,NOEIGEN,MAX
CYC=300) SCF=QC FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radi
cal addition to the C1 (furthest to amine) end of the alkene bond, c\\
0,2\N,-2.3470277375,-0.8314520413,0.4040383032\C,-1.3271267678,1.16616
66648,-0.4851316792\C,0.6344117887,0.0796641554,-0.6650221738\O,1.5714
20705,0.6867582526,0.0484442986\C,2.534065626,-0.1720890145,0.66544233
99\O,0.5204104402,-1.0965774735,-0.8227193716\H,-1.9863377748,-1.33146
19963,-0.3958011923\H,-2.3046026652,-1.3964828814,1.2354346048\H,3.075
2773752,-0.7452571432,-0.0896125972\H,2.0417567235,-0.8644406336,1.351
7341507\H,3.215196537,0.4818403493,1.2070006399\H,-1.0169598881,2.1880
371659,-0.3103592821\H,-1.5099531702,0.8720157018,-1.5115226465\C,-1.8
408714938,0.4374110626,0.5391209916\H,-1.8227070552,0.827550284,1.5526
019137\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-362.1511558\S2=0.79
5121\S2-1=0.\S2A=0.750397\RMSD=0.000e+00\RMSF=2.088e-06\Dipole=0.15921
63,-0.1356014,0.8615066\PG=C01 [X(C4H8N1O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET3\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H8N
1O2(2)\SKYNE\21-Oct-2006\0\\#BHANDHLYP/AUG-CC-PVDZ OPT=(TS,READFC,NOEI
GEN,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radi
cal addition to the C1 (furthest to amine) end of the alkene bond, c\\
0,2\N,-2.4125146679,-0.8154309838,0.4464884843\C,-1.3442627435,1.13637
0187,-0.493301359\C,0.6649031701,0.0828926475,-0.6796922808\O,1.558794
9775,0.6845161963,0.0904451934\C,2.5527717108,-0.164444915,0.683356281
7\O,0.5964497205,-1.0838363572,-0.9128219672\H,-2.1929217154,-1.333487
8853,-0.385695419\H,-2.4084041889,-1.3812035647,1.2728456277\H,3.13461
63395,-0.6601031438,-0.0915555832\H,2.0764705608,-0.9133525638,1.31402
50661\H,3.1840235789,0.4912513237,1.2754188315\H,-1.0037874644,2.14763
02729,-0.3324791276\H,-1.5366120326,0.8315788795,-1.5123241107\C,-1.84
43281015,0.4281863649,0.5492141368\H,-1.782244202,0.8222391493,1.55589
88428\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-362.1823296\S2=0.791
193\S2-1=0.\S2A=0.750376\RMSD=3.296e-09\RMSF=3.765e-06\Dipole=0.092239
2,-0.0952673,0.8906357\PG=C01 [X(C4H8N1O2)]\\@

Transition State 9 (R = CF_3)

UHF/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET10\FTS\UHF\6-311G(d,p)\C5H6F3O2(2)
\SKYNE\29-Oct-2006\0\\#UHF/6-311G** OPT=(TS,READFC,NOEIGEN,MAXCYC=300)
 FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxycyl radical addition to
the C1 (furthest to the trifluoro group) end of the a\\0,2\C,0.7366085
44,1.252782576,-0.8607743144\C,0.5504545974,1.3158509466,1.3737047901\
O,1.1323098717,2.116655648,1.9909440308\H,0.7108236898,2.3255537723,-0
.8975721516\H,1.7059657369,0.8002105382,-0.7659595976\C,-0.3185094428,
0.5330861702,-1.3628325809\H,-1.2587908814,0.9941807863,-1.6031955087\

C,-0.2999385547,-0.9490023331,-1.510444082\F,0.8514595139,-1.4811769906,-1.1488372542\F,-1.243954788,-1.5242916658,-0.7858165541\F,-0.5201634664,-1.3068773194,-2.7653805999\C,-0.4401098884,0.2291045803,3.1804253939\H,-0.8830788477,1.1321136843,3.5768940279\H,-1.1097635939,-0.6071537374,3.2975876892\H,0.5022479657,0.0351820118,3.6734020105\O,-0.2353732389,0.3633562378,1.7713907147\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-640.973264\S2=1.005609\S2-1=0.\S2A=0.760573\RMSD=4.801e-09\RMSF=2.060e-06\Dipole=-0.4190311,0.3299595,0.6257709\PG=C01 [X(C5H6F3O2)]\\@

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FTS\UBHandHLYP\6-311G(d,p)\C5H6F3O2(2)\SKYNE\31-Oct-2006\0\\#BHANDHLYP/6-311G** OPT=(TS,READFC,NOEIGEN,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxycyl radical addition to the C1 (furthest to the trifluoro group) end of the a\\0,2\C,0.7021730009,1.2601389307,-0.9148388099\C,0.567146853,1.3189966068,1.3752387816\O,1.1937435321,2.0691481021,2.0269229314\H,0.6627345981,2.3339990016,-0.9240756217\H,1.6730230374,0.8135826186,-0.7968887561\C,-0.3357148028,0.535631688,-1.3661035927\H,-1.2888818137,0.9759109823,-1.5994366917\C,-0.2915574585,-0.9396245068,-1.494851583\F,0.8971059561,-1.4475639544,-1.1779558304\F,-1.1949679604,-1.5324510791,-0.7104486924\F,-0.566998214,-1.327907168,-2.7429232759\C,-0.4794735709,0.2271898014,3.1476847408\H,-0.8684646996,1.1441517112,3.5713708168\H,-1.1947569951,-0.574659117,3.2419346024\H,0.4556838109,-0.0323943399,3.6268071179\O,-0.2726235451,0.3929411273,1.7330097561\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-643.902044\S2=0.810676\S2-1=0.\S2A=0.750614\RMSD=5.617e-09\RMSF=4.508e-06\Dipole=-0.4119577,0.3926786,0.7728413\PG=C01 [X(C5H6F3O2)]\\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET13\FTS\UBHandHLYP\CC-pVDZ\C5H6F3O2(2)\SKYNE\03-Nov-2006\0\\#BHANDHLYP/CC-PVDZ OPT=(TS,READFC,NOEIGEN,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxycyl radical addition to the C1 (furthest to the trifluoro group) end of the a\\0,2\C,0.7978079509,1.2277378552,-0.944727007\C,0.5834659934,1.3496512702,1.347508417\O,0.9939239546,2.2299005231,2.017248234\H,0.8254985183,2.309291577,-0.9866780686\H,1.7390281258,0.7169299953,-0.7818503692\C,-0.2773696401,0.5502899472,-1.3951274013\H,-1.2030946975,1.0436064316,-1.6679806649\C,-0.3220714824,-0.9308788588,-1.4612766188\F,0.8280118796,-1.4968170425,-1.0963505183\F,-1.2778159686,-1.4335042501,-0.6726324501\F,-0.5969566529,-1.3568805396,-2.6992466271\C,-0.3955186405,0.1465017937,3.0839957501\H,-0.9721378447,1.0050513686,3.4309485956\H,-0.9756273293,-0.7691398905,3.1674568656\H,0.5310562892,0.0714981471,3.6548909581\O,-0.0991441387,0.2885703289,1.6846317913\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-643.7614552\S2=0.810906\S2-1=0.\S2A=0.750612\RMSD=6.243e-09\RMSF=4.880e-06\Dipole=-0.2626275,0.2986374,0.6864887\PG=C01 [X(C5H6F3O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET1\FTS\UBHandHLYP\Aug-CC-pVDZ\C5H6F3O2(2)\SKYNE\03-Nov-2006\0\\#BHANDHLYP/AUG-CC-PVDZ OPT=(TS,READFC,NOEIGEN,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxycyl radical addition to the C1 (furthest to the trifluoro group) end of the a\\0,2\C,0.6258603605,1.2808418138,-0.8780924711\C,0.5509832195,1.2833589349,1.4246188884\O,1.3167367228,1.9345754,2.0455420774\H,0.5278525096,2.3560207426,-0.8406710554\H,1.6238315965,0.878153176,-0.7807205953\C,-0.3863078039,0.5238061618,-1.3469267751\H,-1.3670238388,0.9300872326,-1.553052281\C,-0.270778136,-0.9417434629,-1.5532596831\F,0.9391147742,-1.4185784426,-1.2433248752\F,-1.1617855587,-1.6227875763,-0.8146212692\F,-0.5115053344,-1.2803314238,-2.8304765936\C,-0.5156967296,0.3074077053,3.2560342023\H,-0.7473058989,1.2670603865,3.7128421305\H,-1.3305608731,-0.3954438775,3.3915354077\H,0.4111860425,-0.0874407107,3.6661820217\O,-0.3835817142,0.4685262397,1.8276384284\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-643.8097997\S2=0.809699\S2-1=0.\S2A=0.750621\RMSD=6.132e-09\RMSF=4.568e-06\Dipole=-0.5171398,0.4801498,0.7971645\PG=C0

1 [X(C5H6F3O2)]\\@

Transition State 10 (R = NH_2)

UHF/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET22\FTS\UHF\6-311G(d,p)\C4H8N1O2(2)
\SKYNE\08-Oct-2006\0\\#UHF/6-311G** OPT=(TS,CALCFC,NOEIGEN,MAXCYC=300)
 FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radical addition to
 the C2 (closest to amine) end of the alkene bond, co\\0,2\N,-0.589225
9787,0.2106027405,-2.394651817\C,-0.3145406862,-0.3332476246,0.3921686
803\O,0.5738358163,-0.4488563388,1.3445724366\C,0.0833198104,-0.568193
1274,2.6777554799\O,-1.4828087497,-0.31792871,0.4961212164\C,1.2799758
966,1.2907326717,-1.2644721506\H,-1.1082173324,1.0538610981,-2.2670128
742\H,-1.1999555859,-0.5637813781,-2.2437523441\H,-0.4916647989,0.3083
794394,2.9437878027\H,-0.5365146471,-1.449526571,2.7716692056\H,0.9557
956895,-0.6520221888,3.3064057904\H,0.8621364825,2.2746841888,-1.38899
52365\H,2.2304315129,1.200930508,-0.7747932688\C,0.5537753929,0.156476
354,-1.5879090656\H,1.0691715153,-0.7870735324,-1.6155532436\\Version=
x86-Linux-G03RevB.04\State=2-A\HF=-360.3056332\S2=0.98629\S2-1=0.\S2A=
0.759452\RMSD=6.319e-09\RMSF=1.902e-06\Dipole=0.2749681,-0.0508576,0.7
476828\PG=C01 [X(C4H8N1O2)]\\@

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET2\FTS\UBHandHLYP\6-311G(d,p)\C4H8N
1O2(2)\SKYNE\08-Oct-2006\0\\#BHANDHLYP/6-311G** OPT=(TS,READFC,NOEIGEN
,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radical
 addition to the C2 (closest to amine) end of the alkene bond, co\\0,2
\N,-0.6002930065,0.2216793336,-2.3742602781\C,-0.2886206126,-0.3724233
689,0.3654899453\O,0.5980202289,-0.5078135853,1.3272000136\C,0.0807333
304,-0.5402177891,2.6638913392\O,-1.4618624829,-0.2756320958,0.4810295
617\C,1.237801873,1.2810732036,-1.206084688\H,-1.1451194172,1.04928526
25,-2.2173260599\H,-1.1846442326,-0.5860294482,-2.271353714\H,-0.44267
60624,0.3824448023,2.8821224772\H,-0.5977237909,-1.3758996836,2.782561
4885\H,0.9392015946,-0.652711321,3.3088119569\H,0.8028728119,2.2631427
048,-1.280743889\H,2.1967394817,1.18424972,-0.7347575975\C,0.548914469
9,0.168729038,-1.6010233049\H,1.0711643272,-0.7716384255,-1.6489690671
\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-362.2250432\S2=0.815802\S
2-1=0.\S2A=0.75066\RMSD=6.770e-09\RMSF=3.035e-07\Dipole=0.1407229,-0.0
857188,0.6117421\PG=C01 [X(C4H8N1O2)]\\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET16\FTS\UBHandHLYP\CC-pVDZ\C4H8N1O2
(2)\SKYNE\08-Oct-2006\0\\#BHANDHLYP/CC-PVDZ OPT=(TS,READFC,NOEIGEN,MAX
CYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radical add
ition to the C2 (closest to amine) end of the alkene bond, co\\0,2\N,-
0.64113867,0.2636554532,-2.3375558901\C,-0.2572841296,-0.3910637634,0.
3678121717\O,0.60497029,-0.4113125542,1.363471823\C,0.0390291635,-0.51
75570459,2.675440101\O,-1.4419211986,-0.4454731124,0.4429880838\C,1.28
41558143,1.2807656967,-1.2551789776\H,-1.134838934,1.1274906726,-2.164
4442213\H,-1.2658250797,-0.4991915328,-2.1200497454\H,-0.6251935434,0.
3266085764,2.8687140084\H,-0.5246877221,-1.447258637,2.7710390535\H,0.
8809735163,-0.508480423,3.3645434448\H,0.866204711,2.2811803379,-1.302
0281332\H,2.2719819122,1.1559704766,-0.832752399\C,0.545836113,0.18586
69966,-1.6188865831\H,1.0445413307,-0.7756936143,-1.6889303034\\Versio
n=x86-Linux-G03RevB.04\State=2-A\HF=-362.1470617\S2=0.816837\S2-1=0.\S
2A=0.750676\RMSD=9.222e-09\RMSF=2.194e-06\Dipole=0.110298,-0.0066063,0
.6583372\PG=C01 [X(C4H8N1O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET18\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H8
N1O2(2)\SKYNE\08-Oct-2006\0\\#BHANDHLYP/AUG-CC-PVDZ OPT=(TS,READFC,NOE
IGEN,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl rad
ical addition to the C2 (closest to amine) end of the alkene bond, co\
\0,2\N,-0.5588322729,0.1691232045,-2.4227971786\C,-0.3208137133,-0.340

8133648,0.3756642815\O,0.5809497172,-0.595861773,1.3046776594\C,0.1111
372349,-0.5826419729,2.6627690751\O,-1.4748667275,-0.1049339208,0.5377
116935\C,1.2005800141,1.2919623007,-1.1878394813\H,-1.1424285365,0.978
6298669,-2.3005848158\H,-1.1148268495,-0.6650798886,-2.3670703392\H,-0
.2912152896,0.3989795471,2.906025962\H,-0.6608354112,-1.3375678026,2.7
988904663\H,0.9791395866,-0.8056944819,3.2751944511\H,0.7453136944,2.2
673438819,-1.2994281073\H,2.1472548219,1.2230698746,-0.6752394264\C,0.
5589485654,0.1554220377,-1.6029559422\H,1.1016473703,-0.7807518831,-1.
6031503626\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-362.1772305\S2=
0.813733\S2-1=0.\S2A=0.750648\RMSD=9.721e-09\RMSF=2.123e-06\Dipole=0.2
247717,-0.1667602,0.5049167\PG=C01 [X(C4H8N1O2)]\\@

Transition State 10 (R = CF_3)

UHF/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET1\FTS\UHF\6-311G(d,p)\C5H6F3O2(2)\
SKYNE\29-Oct-2006\0\\#UHF/6-311G** OPT=(TS,READFC,NOEIGEN,MAXCYC=300)
FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radical addition to
the C2 (closest to the trifluoro group) end of the a\\0,2\C,0.69812015
09,0.8733370975,0.6482443837\H,0.6340843085,0.7779694098,1.7169014671\
H,1.984650927,1.3415309016,-0.9999905586\H,2.8291785342,0.9023162965,0
.5774406553\C,1.9173000005,1.0864750412,0.0407202377\O,0.3716609727,-1
.9891786904,1.4616332059\C,0.3148868337,-1.3337703947,0.4985184016\C,-
0.5554502836,1.4062314139,0.0173750788\F,-1.6293209564,0.7455118171,0.
4090284089\F,-0.7459702251,2.6704430943,0.3579052401\F,-0.5180910619,1
.3602038188,-1.2979206548\C,0.1693289982,-3.0882293353,-1.0239403039\H
,-0.7088994101,-3.5138129417,-0.5590867411\H,0.1085277277,-3.170738599
2,-2.096906355\H,1.0570738694,-3.5810256966,-0.652501172\O,0.237177781
6,-1.6865626693,-0.7481933348\\Version=x86-Linux-G03RevB.04\State=2-A\
HF=-640.9696033\S2=1.032006\S2-1=0.\S2A=0.762138\RMSD=7.027e-09\RMSF=4
.671e-06\Dipole=0.7786786,-0.6898553,-0.5534521\PG=C01 [X(C5H6F3O2)]\\
@

BHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FTS\UBHandHLYP\6-311G(d,p)\C5H6F
3O2(2)\SKYNE\02-Nov-2006\0\\#BHANDHLYP/6-311G** OPT=(TS,READFC,NOEIGEN
,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radical
 addition to the C2 (closest to the trifluoro group) end of the a\\0,2
\C,-1.1619972805,0.5578219013,0.2657162736\H,-1.210856633,0.9429862844
,1.2692011292\H,-1.6437317115,0.8645078571,-1.7709557255\H,-1.75061504
95,2.348341812,-0.6837001465\C,-1.5658554365,1.2947338125,-0.789057944
6\O,1.5488196634,1.4574892915,1.3014737525\C,1.0850134066,0.8651320947
,0.3990838352\C,-1.1652200023,-0.9363946478,0.1899061131\F,-0.27790225
8,-1.4917589759,1.0130905861\F,-2.3592914746,-1.4175603066,0.543393355
5\F,-0.9101662254,-1.3832073892,-1.0345183318\C,3.0048370921,0.8626735
906,-0.9182411415\H,3.6082527997,0.3683156035,-0.1679476228\H,3.262832
7557,0.5151038754,-1.9064574095\H,3.128705044,1.9353195813,-0.84150313
47\O,1.6200535541,0.516806274,-0.7365700516\\Version=x86-Linux-G03RevB
.04\State=2-A\HF=-643.8977071\S2=0.820368\S2-1=0.\S2A=0.750721\RMSD=1.
178e-09\RMSF=9.315e-06\Dipole=-0.4449703,-0.826732,-0.8006462\PG=C01 [
X(C5H6F3O2)]\\@

BHandHLYP/cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FTS\UBHandHLYP\CC-pVDZ\C5H6F3O2(
2)\SKYNE\30-Oct-2006\0\\#BHANDHLYP/CC-PVDZ OPT=(TS,READFC,NOEIGEN,MAXC
YC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radical addi
tion to the C2 (closest to the trifluoro group) end of the a\\0,2\C,0.
7365744676,0.9071576576,0.6436448202\H,0.6908169669,0.7936843907,1.720
5682948\H,1.9476688048,1.3128696652,-1.0543369021\H,2.8532661962,0.890
5428342,0.513173343\C,1.9157727345,1.0706601804,0.0010666421\O,0.27722
78967,-2.0136597341,1.4694544594\C,0.2715679129,-1.3244027766,0.512044
3191\C,-0.5356759919,1.3998237408,0.0274042456\F,-1.6020596405,0.70370
94095,0.4251630462\F,-0.7637418609,2.669491281,0.3776894168\F,-0.50428
75459,1.3594750762,-1.3020281141\C,0.1968518023,-3.0623767853,-1.03142

73044\H,-0.7240802485,-3.4826943352,-0.6250100499\H,0.2132095996,-3.14
89541796,-2.1152301615\H,1.0567147274,-3.5670754449,-0.5885339772\O,0.
2581045816,-1.6535436324,-0.7537602123\\Version=x86-Linux-G03RevB.04\S
tate=2-A\HF=-643.7574001\S2=0.820902\S2-1=0.\S2A=0.750727\RMSD=9.216e-
09\RMSF=5.349e-06\Dipole=0.7465786,-0.723287,-0.5137098\PG=C01 [X(C5H6
F3O2)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET2\FTS\UBHandHLYP\Aug-CC-pVDZ\C5H6F
3O2(2)\SKYNE\01-Nov-2006\0\\#BHANDHLYP/AUG-CC-PVDZ OPT=(TS,READFC,NOEI
GEN,MAXCYC=300) FREQ=NORAMAN GEOM=CHECKPOINT GUESS=CHECK\\Oxyacyl radi
cal addition to the C2 (closest to the trifluoro group) end of the a\\
0,2\C,0.7249644826,0.8952494665,0.6457706664\H,0.6644908551,0.75569387
13,1.7160566752\H,1.9688357689,1.3405670364,-1.0199958002\H,2.83943434
93,0.8650752919,0.5448745918\C,1.9143212363,1.0658421022,0.0236737519\
O,0.3301202175,-2.0036763207,1.4634213349\C,0.273736,-1.3364563105,0.4
895680459\C,-0.5375239857,1.414166564,0.028042565\F,-1.6221580777,0.73
93671528,0.4258767921\F,-0.7423972178,2.6930977156,0.3829726114\F,-0.5
121351384,1.3806350869,-1.3055988851\C,0.1935997945,-3.107794728,-1.02
71043246\H,-0.6970810918,-3.5425454301,-0.5788800141\H,0.1684255631,-3
.2018397578,-2.1074811333\H,1.0846867128,-3.5763897346,-0.6148425202\O
,0.2257343553,-1.6893866093,-0.7670076715\\Version=x86-Linux-G03RevB.0
4\State=2-A\HF=-643.8051041\S2=0.819586\S2-1=0.\S2A=0.750727\RMSD=8.89
4e-09\RMSF=2.398e-06\Dipole=0.8106099,-0.7462856,-0.5546866\PG=C01 [X(
C5H6F3O2)]\\@