

Mechanistic insights into ozone-initiated oxidative degradation of saturated hydrocarbons and polymers

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Supporting Information

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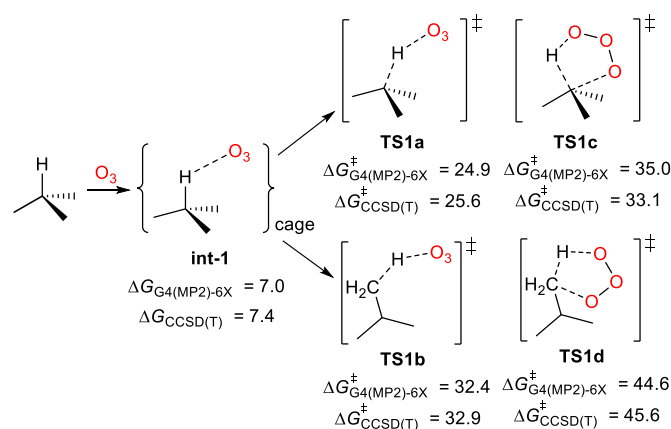
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Detailed computational information

All calculations were carried out with the Gaussian 09¹ computational suite as mentioned in the computational methods section of main manuscript. Geometry optimization of minimum and transition state structures were performed with Truhlar's M11 functional² and Pople's double ζ 6-31+G(d,p) basis set^{3, 4}. Electronic energies were further improved with highly-correlated techniques including the composite G4(MP2)-6X method⁵ and benchmark calculations with restricted coupled cluster theory RCCSD(T)⁶ and Aldrich's triple ζ def2-TZVP basis set⁷ (see Schemes S1 and S2). The G4(MP2)-6X composite method introduced by Chan and Radom constitutes a series of single-point energy calculations and this composite method was reported to perform close to the G4 level.⁵ Thermal and entropic corrections (at 298.15K) were calculated using the standard textbook formulae for the statistical thermodynamics of an ideal gas under the harmonic oscillator / rigid rotor approximation, and combined with G4(MP2)-6X and RCCSD(T) electronic energies to obtain the Gibbs' free energies.

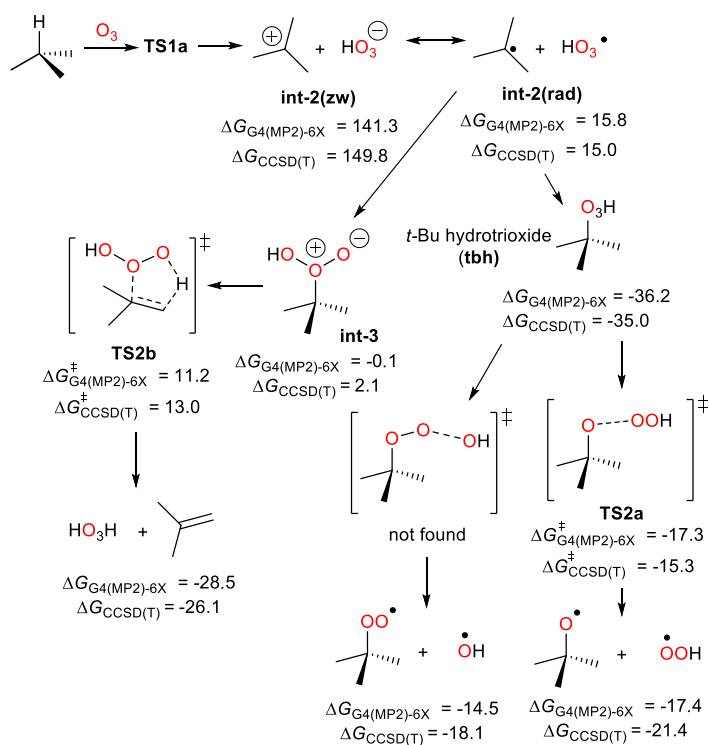
RCCSD(T) and G4(MP2)-6X benchmark studies

In scheme S1, G4(MP2)-6X and RCCSD(T) free energies for the first O₃ C-H bond oxidation elementary step were compared and were found to agree to within 2 to 1 kcal/mol.



Scheme S1. Benchmark for RCCSD(T) and G4(MP2)-6X. Reaction and activation free energies in kcal/mol relative to starting materials for 1st H...O₃ abstraction.

The free energy comparison was subsequently carried out for the following oxidation-decomposition process in Scheme S2. Both computational methods show good agreement in terms of reaction free energies (ΔG) and free energy barriers (ΔG[‡]) with respect to the starting materials isobutane and ozone. G4(MP2)-6X thus demonstrates excellent accuracy at a much lower computational cost and is suitable to model larger molecules.



Scheme S2. Reaction and activation free energies RCCS(T) and G4(MP2)-6X comparison in kcal/mol for subsequent decomposition processes.

Table S1. Summary of electronic energies at G4(MP2)-6X and RCCSD(T) for isobutane and corrections at M11/6-31+G(d,p) level of theory^a

Molecule	E[G4(MP2)-6X]	E[R-CCSD(T)]	G _{correction}	H _{correction}	ZPE
O₃ (UM11)	-225.2517173	-225.1412077	-0.01673	0.010977	0.007063
O₃ (RM11)	-225.25027794	-225.1394687	-0.01561	0.011986	0.008108
isobutane	-158.2836887	-158.1307522	0.104285	0.137582	0.130898
³O₂	-150.2056407	-150.1345427	-0.01593	0.007322	0.004016
¹O₂	-150.159155	-150.086214	-0.01491	0.007306	0.004
int-1	-383.5387362	-383.2746868	0.102075	0.150627	0.139233
TS1a	-383.5063889	-383.2419171	0.098268	0.14397	0.133301
TS1b	-383.4938832	-383.2335612	0.101868	0.144834	0.1349
TS1c	-383.4938553	-383.2296506	0.097681	0.143819	0.13337
TS1d	-383.4799593	-383.2149485	0.103198	0.146117	0.136529
tBu*	-157.614228	-157.4689203	0.086553	0.1235	0.116114
HOOO*	-225.8874482	-225.770615	-0.00759	0.022959	0.018166
tBu+	-157.3618133	-157.2205982	0.088873	0.122653	0.116313
HOOO-	-225.9402596	-225.8045867	-0.00943	0.020003	0.015427
tbh	-383.6160309	-383.3506463	0.110473	0.152522	0.142811
TS2a	-383.5812724	-383.3147384	0.105932	0.149712	0.139445
alkoxyl	-232.7702003	-232.5898378	0.092402	0.129492	0.12199
HOO*	-150.7901973	-150.713561	-0.00757	0.018377	0.014581
peroxyl	-307.8811861	-307.6639603	0.095793	0.135499	0.127047
HO*	-75.677227	-75.6367208	-0.00834	0.011893	0.008589
int-3	-383.5575773	-383.29051	0.109529	0.15157	0.141778
TS2b	-383.5356645	-383.2694243	0.105726	0.14727	0.137802
alkene*	-157.0493747	-156.9078822	0.080023	0.113764	0.107434
HO₃H	-226.530163	-226.4044792	0.006291	0.035797	0.031073

TS3	-232.7568672	-	0.087749	0.126093	0.118094
TS4b	-383.563509	-	0.097626	0.144248	0.133715
TS4c	-391.0461229	-	0.209871	0.263302	0.249086
CH₃COCH₃	-192.9673228	-	0.056465	0.088932	0.083401
CH₃*	-39.7918915	-	0.010446	0.033636	0.029609
CH₃COO*	-190.0520411	-	0.017639	0.048133	0.04335
CH₃OOH	-190.702887	-	0.028954	0.060505	0.055049
H2O assisted C-H bond oxidation					
int-1w	-459.9236133	-	0.120923	0.178128	0.162882
TS1aw	-459.8956889	-	0.117653	0.171783	0.157535

^a All values are in Hatrees.

Table S2. Summary of electronic energies at G4(MP2)-6X and RCCSD(T) for polymers and corrections at M11/6-31+G(d,p) level of theory^a

Molecule	E[G4(MP2)-6X]	G _{correction}	H _{correction}	ZPE
Poly(propylene)				
pProp	-276.0959135	0.182169	0.225993	0.215494
int-1	-501.3511314	0.182176	0.239344	0.224161
TS1a	-501.3184509	0.178232	0.232697	0.218311
TS1b	-501.3151361	0.179221	0.232805	0.21856
int-2(rad)	-275.4275169	0.166026	0.212255	0.201204
hydrotrioxide	-501.4266482	0.190211	0.241294	0.227756
TS2a	-501.3936548	0.186504	0.238658	0.224717
alkoxyl	-350.5836698	0.172285	0.21825	0.207036
TS3a	-350.5748085	0.168171	0.21548	0.203859
TS4(1,4)	-350.5542614	0.167167	0.213081	0.202053
TS4(1,5)	-350.5639597	0.168234	0.212684	0.20221

ROOH	-308.5184502	0.108234	0.148155	0.1397
Poly(styrene)				
pSty	-659.1055388	0.279753	0.33931	0.322957
int-1	-884.3609367	0.277858	0.352478	0.331085
TS1a	-884.3307269	0.277499	0.346096	0.325845
TS1b	-884.3222686	0.274275	0.345535	0.325048
int-2(rad)	-658.4886002	0.263775	0.325935	0.309209
hydrotrioxide	-884.4308671	0.288034	0.354589	0.335055
TS2a	-884.4000994	0.281453	0.35162	0.331284
alkoxyl	-733.5906644	0.267107	0.331192	0.313716
TS3a	-733.5887919	0.263613	0.3287	0.310963
CH₃COR¹	-384.4721527	0.105369	0.146805	0.138063
ROOH	-500.0227548	0.155474	0.204528	0.192968
Poly(methyl acrylate)				
pMA	-652.9095891	0.205692	0.26367	0.247666
int-1	-878.1655805	0.20567	0.276711	0.255939
TS1a	-878.1271106	0.20124	0.269718	0.249651
TS1b	-878.1245935	0.202414	0.270094	0.250246
int-2(rad)	-652.2518851	0.189014	0.250009	0.233439
hydrotrioxide	-878.2342483	0.214004	0.278442	0.259314
TS2a	-878.2027363	0.207877	0.275299	0.255451
alkoxyl	-727.3922232	0.194801	0.255173	0.238259
TS3a	-727.3884112	0.191885	0.252579	0.235485
TS3b	-727.3903831	0.192334	0.253273	0.236186
CH₃COR¹	-381.3571702	0.066705	0.1084	0.099574
ROOH	-496.9223281	0.118295	0.16657	0.155132
CH₃COR	-499.1877112	0.146117	0.197305	0.184514
MeOC(O)*	-228.1962884	0.022194	0.055059	0.049608
Poly(methyl methacrylate)				

pMMA	-731.4524522	0.260467	0.321866	0.303476
int-1	-956.7075732	0.259576	0.334919	0.311635
TS1a	-956.6680377	0.256551	0.328126	0.305771
TS1b	-956.6617284	0.255709	0.327913	0.30563
int-2(rad)	-730.7804554	0.243982	0.307598	0.288689
hydrotrioxide	-956.7681167	0.266731	0.337615	0.316036
TS2a	-956.7459715	0.264923	0.334299	0.312462
alkoxyl	-805.9367884	0.249716	0.313522	0.294321
TS3a	-805.9280227	0.247298	0.311741	0.292351
CH₃COR¹	-459.9041874	0.119631	0.167353	0.155891
ROOH	-496.9311446	0.119403	0.166533	0.154997
Poly(vinyl chloride)				
pVC	-1115.902945	0.108512	0.152488	0.142788
int-1	-1341.161369	0.10939	0.164459	0.150811
TS1b	-1341.116469	0.104468	0.158417	0.144836
TS1a	-1341.117936	0.104067	0.158501	0.144814
int-2(rad)	-1115.23479	0.093029	0.138723	0.128671
hydrotrioxide	-1341.227407	0.11574	0.166943	0.154102
TS2a	-1341.199448	0.112139	0.1644	0.151262
alkoxyl	-1190.373457	0.096936	0.143728	0.133039
acetone+Cl*	-1190.396785	0.094593	0.144836	0.133219
Cumene				
cumene	-349.7872886	0.150873	0.194164	0.184536
TS(1,3dipolar)	-575.0183011	0.156958	0.207031	0.194651
primary ozonide	-575.0761804	0.16122	0.209938	0.198109
TS1(sp²) step-wise	-574.9882737	0.14619	0.200034	0.186326
TS1(sp²) concerted	-575.004643	0.156024	0.205173	0.192945

int-1	-575.0413023	0.149898	0.207169	0.19278
TS1a	-575.0133233	0.147982	0.200789	0.18744
int-1w	-651.4269977	0.168078	0.234722	0.216411
TS1aw	-651.4031354	0.167257	0.228938	0.211962
Methyl isobutyrate				
ester	-346.688496	0.113379	0.15626	0.146699
TS1b	-571.8974038	0.108886	0.162467	0.149291
int-1	-571.9441978	0.111641	0.169199	0.154751
TS1a	-571.906842	0.10955	0.162444	0.14903
int-1w	-648.3378997	0.135541	0.197238	0.180026
TS1aw	-648.2970162	0.130475	0.1903	0.173648

^a All values are in Hatrees.

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Gaussian Archive Files

isobutane

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isobutane

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027496702,-0.657092421,-0.4071585914\C,1.4226515575,0.3159023291,0.571
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31+G** opt scf=maxcyc=200 # int=ultrafine freq\O2 (triplet; sigma sym
m)\0,3\O,-0.9915000146,-0.5791204217,0.0024636059\O,-0.8727889854,0.6
114364217,0.0011943941\Version=ES64L-G09RevD.01\State=3-SGG\HF=-150.2
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```

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G** opt scf=maxcyc=200 guess=mix # int=ultrafine freq\O2 (singlet; de
lta symm)\0,1\O,0.,0.,0.5986248719\O,0.,0.,-0.5986248719\Version=ES6
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358e-09\RMSF=6.713e-05\Dipole=0.,0.,0.\Quadrupole=0.1372345,0.1372345,
-0.274469,0.,0.,0.\PG=D*H [C*(O1.O1)]\@
```

int-1

```
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/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman # gu
ess=read geom=allcheck int=ultrafine\Cage 1 intm - isobutane + ozone
'diradical'\0,1\C,2.151987675,-0.9400724649,0.0856225499\H,3.08988525
89,-0.6702665083,-0.4250565116\C,1.427379305,0.3198072248,0.568344769\
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\H,1.533044711,-1.5089657879,-0.623740498\C,1.0777486835,1.226254311,-
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TS1a

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6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200)
freq=noraman nosymm # guess=read geom=allcheck int=ultrafine\\TS for O
3 sec-H abs of isobutane\\0,1\C,2.3531330292,-0.6822300598,0.018041885
4\H,3.2773928187,-0.1154750242,0.2203054283\C,1.1551420152,0.127349875
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577751,1.3822296081,-0.3352550372\H,1.7889460406,2.042579566,-0.266377
2523\H,0.7533208547,1.145018845,-1.3975435946\H,0.036742771,1.94042646
81,0.0308227757\C,1.0845789121,0.3331583479,1.9846085046\H,1.926300884
8,0.9697088157,2.306117848\H,0.1484676341,0.8272362923,2.2749992238\H,
1.1594702786,-0.6202281963,2.5243350765\\Version=ES64L-G09RevE.01\HF=-
383.6634345\S2=0.760129\S2-1=0.\S2A=0.040475\RMSD=9.598e-09\RMSF=1.344
e-05\Dipole=1.160038,0.2693572,0.0408021\Quadrupole=-0.4226648,-0.1850
827,0.6077475,0.251036,1.255176,-0.3126791\PG=C01 [X(C4H10O3)]\@

TS1b

1\1\GINC-R126\FTS\RM11\6-31+G(d,p)\C4H10O3\ROOT\11-May-2016\0\#\ m11/6
-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200) f
req=noraman int=ultrafine\\TS for O3 alpha sec-H abs of isobutane 'zwi
tterionic'\\0,1\C,2.0968096056,-0.7454497207,0.1213604063\H,3.06386330
03,-0.2563601306,0.3329238127\C,0.9861697253,0.2202625638,0.4890002839
\H,2.0564332414,-1.6660311059,0.7189917275\O,-1.7610630604,0.529055742
1,0.6095404683\O,-1.6793453601,-0.0602475741,-0.5388800174\O,-0.953132
6889,-1.1628823131,-0.3935389821\H,-0.0601468369,-0.696706737,0.149618
6\H,2.0759006741,-1.0072023987,-0.9443357892\C,0.7686682098,1.34139580
67,-0.4759382514\H,0.3064388902,2.2067623588,0.0139305868\H,1.71018540
54,1.6247925633,-0.972014438\H,0.0701696958,1.0344246202,-1.2806633139
\C,0.8377827498,0.4693858476,1.968282127\H,0.1256176281,1.2767978336,2
.1651590542\H,0.4811508551,-0.4303315378,2.4905253314\H,1.8247515356,0
.7228847918,2.3945127838\\Version=ES64L-G09RevE.01\State=1-A\HF=-383.6
389478\RMSD=9.600e-09\RMSF=8.692e-06\Dipole=1.6419957,0.1166978,0.0508
984\Quadrupole=-1.4022866,0.2632036,1.139083,0.0613595,0.7039998,-0.88
24369\PG=C01 [X(C4H10O3)]\@

TS1c

1\1\GINC-R112\FTS\UM11\6-31+G(d,p)\C4H10O3\ROOT\11-May-2016\0\#\ um11/
6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200)
freq=noraman nosymm # guess=read geom=allcheck int=ultrafine\\TS for O
3 alpha pri-H abs of isobutane\\0,1\C,-2.2169603974,0.7176122155,-0.48
31126047\H,-2.8558316505,0.9994942919,0.3682842174\C,-1.6069960337,-0.
6694336612,-0.2589898305\H,-1.4347695817,1.4808660229,-0.5949257351\C,
-0.7529896291,-0.6906251128,0.988849673\H,-0.157351416,-1.5974170608,1
.1520103902\H,0.1417124657,0.2121500697,0.8195456331\O,1.8047379922,-0
.4804355678,-0.9281820611\O,2.0794653751,0.169602139,0.1282313321\O,1.
0684891243,1.0094518941,0.49343875\H,-0.9644517328,-0.9198930647,-1.11
65826027\H,-1.2523202427,-0.3432732882,1.9038603656\H,-2.8387567659,0.
7289729129,-1.3885761122\C,-2.7054814718,-1.7411371714,-0.1350350074\H
, -3.3212810724,-1.7597390085,-1.0450907873\H,-2.2802700951,-2.74334893
48,0.0116042486\H,-3.3666230984,-1.5200518958,0.7163129011\\Version=ES
64L-G09RevE.01\HF=-383.6534436\S2=0.822628\S2-1=0.\S2A=0.051476\RMSD=9
.276e-09\RMSF=1.586e-06\Dipole=-0.9627577,-0.4225768,0.3757911\Quadrup
ole=-0.3737807,-0.1294927,0.5032734,0.4575993,0.4666496,-1.0375242\PG=
C01 [X(C4H10O3)]\@

TS1d

1\1\GINC-R130\FTS\RM11\6-31+G(d,p)\C4H10O3\ROOT\11-May-2016\0\#\ m11/6-31+g(d,p) opt=(ts,calcf, noeigen,maxcyc=200) scf=(tight,maxcyc=200) freq=noraman int=ultrafine\TS for O3 alpha pri-H abs of isobutane 'zwittrionic'\0,1\C,-1.8872371741,0.9256777371,-0.3124727219\H,-2.1118531378,1.4038807505,0.6544666278\C,-1.6477439643,-0.5766618659,-0.1224573807\H,-1.0013697749,1.4129586703,-0.7412021408\C,-0.4884523764,-0.8127712379,0.8177489886\H,-0.0648471886,-1.8187823362,0.8287066671\H,0.4078096144,0.2510950644,0.8401697674\O,1.0103674105,-0.5222481191,-0.8788140734\O,1.938489345,0.0026214837,-0.1678149678\O,1.3737940413,0.955667153,0.550653807\H,-1.3938925237,-1.0182346734,-1.0969938057\H,-0.7026020748,-0.4803772303,1.8507155693\H,-2.7404622914,1.10406206,-0.9809821716\C,-2.9052291308,-1.2699436786,0.4264657236\H,-3.7473406327,-1.1396384211,-0.267481023\H,-2.7446716284,-2.3471581701,0.5710074956\H,-3.1968706631,-0.8347216066,1.3941897986\Version=ES64L-G09RevE.01\State=1-A\HF=-383.6289189\RMSD=6.336e-09\RMSF=3.807e-05\Dipole=-0.790008,-0.3484999,0.4247164\Quadrupole=-0.8897278,0.0642369,0.825491,-0.673708,0.4426682,-0.8655736\PG=C01 [X(C4H10O3)]\@\

tBu*

1\1\GINC-R2868\FOpt\UM11\6-31+G(d,p)\C4H9(2)\ROOT\21-May-2016\0\#\ m11/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm int=ultrafine\ tBu*\0,2\C,0.2953022799,-0.5720545438,-0.2735046495\C,0.8886605054,-1.9082903326,0.0424317354\H,0.47700855,-2.3247466147,0.9730954255\H,0.6768270645,-2.6444187093,-0.7586398454\H,1.9823490228,-1.8529213269,0.1414841461\C,0.9957671475,0.3009173706,-1.2657894627\H,0.6538741694,1.3439293417,-1.2003841255\H,2.0858070443,0.2837702534,-1.1223566092\H,0.8045499977,-0.0339090955,-2.3049158853\C,-1.1737721079,-0.379279066,-0.0683993875\H,-1.5175194501,-0.8477712583,0.8650780086\H,-1.4426487323,0.6865566011,-0.0408390678\H,-1.760306551,-0.8359484099,-0.8905314127\Version=ES64L-G09RevE.01\HF=-157.6869665\S2=0.753443\S2-1=0.\S2A=0.75001\RMSD=2.422e-09\RMSF=2.840e-05\Dipole=-0.0384581,-0.0593964,-0.1034543\Quadrupole=0.0579309,0.1393565,-0.1972874,-0.0920459,-0.2125156,-0.1273975\PG=C01 [X(C4H9)]\@\

H000*

1\1\GINC-R2413\FOpt\UM11\6-31+G(d,p)\H1O3(2)\ROOT\21-May-2016\0\#\ m11/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm int=ultrafine\H000*\0,2\O,-0.513163155,-1.0022714882,0.000000283\H,-0.6864589066,-0.0449357966,-0.000000929\O,0.9453783499,-0.9985457595,0.000002136\O,1.3602788617,-2.1732970256,0.000020211\Version=ES64L-G09RevE.01\HF=-225.9789802\S2=0.753317\S2-1=0.\S2A=0.750008\RMSD=3.561e-09\RMSF=1.127e-04\Dipole=-0.3058377,0.9999808,-0.0000005\Quadrupole=0.6260807,-1.8335699,1.2074892,0.0854095,-0.000001,0.0000026\PG=C01 [X(H1O3)]\@\

tBu⁺

1\1\GINC-R426\FOpt\RM11\6-31+G(d,p)\C4H9(1+)\ROOT\21-May-2016\0\#\ m11/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm int=ultrafine\ tBu+\1,1\C,0.2460726372,-0.6567458074,-0.4319445829\C,0.9809100554,-1.790896523,0.1280065165\H,0.5991013493,-2.0928420515,1.1120949443\H,0.7346987234,-2.6341148826,-0.5532000732\H,2.0681785242,-1.6661693021,0.119470499\C,0.8867126666,0.2513180042,-1.3824460465\H,0.3900698687,1.2268878601,-1.4465076979\H,1.9701950446,0.3364579076,-1.2457468822\H,0.7270078329,-0.2408944062,-2.3669322642\C,-1.1560099473,-0.4567305211,-0.0727302381\H,-1.6533448557,-1.366686296,0.2822786961\H,-1.0972605454,0.2343777038,0.7974363338\H,-1.7304324139,0.0718725341,-0.8430502946\Version=ES64L-G09RevE.01\HF=-157.4372892\RMSD=6.388e-09\RMSF=2.677e-06\Dipole=-0.043669,-0.0473573,-0.0548369\Quadrupole=-0.2041095,0.9661111,-0.7620015,-1.4394275,-1.578949,-0.4022469\PG=C01 [X(C4H9)]\@\

H000⁻

1\1\GINC-R3442\FOpt\RM11\6-31+G(d,p)\H1O3(1-)\ROOT\21-May-2016\0\#\ m11/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm int=ultrafine\H000-\1,1\O,-0.6844667786,-0.9634318411,-0.0000351467\H,-0.7259266792,0.0026516855,0.0000406892\O,1.0518828785,-1.0189192651,-0.0000367129\O,1.4645457293,-2.2393506493,0.0000333404\Version=ES64L-G09RevE.01\HF=-226.029293\RMSD=4.129e-09\RMSF=1.523e-04\Dipole=

-0.0423275,1.0708941,0.0000324\Quadrupole=0.3938174,-5.692944,5.299126
6,4.7014881,-0.0002111,0.0000961\PG=C01 [X(H1O3)]\@

tbh

1\1\GINC-R114\FOpt\RM11\6-31+G(d,p)\C4H10O3\ROOT\11-May-2016\0\#\# m11/
6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman int=u
ltrafine\Intm 2 trioxide - secondary H abstr.\0,1\C,-0.6547118681,1.
4974989882,-0.0827945373\H,-1.5964351875,2.0434679088,-0.2345748673\C,
-0.9615097555,0.1157658756,0.4884581077\H,-0.0178391162,2.0670353662,0
.6063325759\O,0.2741304522,-0.5825908559,0.8234644081\O,1.0607916205,-
0.7322966414,-0.328606057\O,2.0048030282,0.3140429406,-0.3294317445\H,
2.7031070048,-0.0360328096,0.2471040115\H,-0.1371838165,1.4173879604,-
1.047119495\C,-1.7619354332,-0.7357738912,-0.4940323545\H,-1.953235257
5,-1.730167809,-0.0688732903\H,-2.7249905162,-0.2530242361,-0.71063562
51\H,-1.2121424969,-0.8524659133,-1.4367253958\C,-1.6543590655,0.20952
03474,1.8446164234\H,-1.0501299632,0.8003963166,2.5454209913\H,-2.6317
7285,0.6956591896,1.7244672171\H,-1.8089361796,-0.7918917767,2.2674938
816\Version=ES64L-G09RevE.01\State=1-A\HF=-383.7812693\RMSD=7.063e-09
\RMSF=6.187e-06\Dipole=-0.2341501,0.2171142,0.31686\Quadrupole=4.04070
75,-2.0278498,-2.0128577,-0.5535801,1.6096586,0.5071278\PG=C01 [X(C4H1
0O3)]\@

TS2a

1\1\GINC-R144\FTS\UM11\6-31+G(d,p)\C4H10O3\ROOT\11-May-2016\0\#\# um11/
6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200)
freq=noraman nosymm # guess=read geom=allcheck int=ultrafine\TS for t
ert-CO---OOH cleavage\0,1\C,-0.6403924823,1.3991242736,0.0222998008\H
, -1.4253340818,2.074236147,0.3917820432\C,-0.9546949893,-0.0482268787,
0.4144169146\H,0.3205677234,1.7091307564,0.4528775203\O,-0.0702969116,
-0.9428617276,-0.1978280099\O,1.7959365584,-0.3726139077,0.490527312\O
,2.3249904611,0.2999770329,-0.5142054997\H,2.7400213426,-0.3704632393,
-1.0864763\H,-0.5778822217,1.4878830565,-1.0706717648\C,-2.3165950415,
-0.4805214251,-0.1802832004\H,-2.528549185,-1.5283062456,0.0666554085\
H,-3.1013883607,0.1559322986,0.250882254\H,-2.3161623962,-0.3593822089
, -1.2708556606\C,-0.9518823502,-0.2398308711,1.9338919534\H,0.03626231
29,0.0166332724,2.3377878809\H,-1.70388296,0.4086018428,2.4055341596\H
, -1.1743232883,-1.2857206864,2.1832803481\Version=ES64L-G09RevE.01\HF
=-383.7389648\S2=0.791885\S2-1=0.\S2A=0.022397\RMSD=2.928e-09\RMSF=2.5
27e-06\Dipole=-0.04989,0.1426274,-0.3268845\Quadrupole=3.7887498,-3.36
99144,-0.4188354,-1.6224616,-3.5525253,0.7677753\PG=C01 [X(C4H10O3)]\@
@

tBuO*

1\1\GINC-R2861\FOpt\UM11\6-31+G(d,p)\C4H9O1(2)\ROOT\21-May-2016\0\#\# m
11/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman no
symm int=ultrafine\TBuO*\0,2\C,0.9420208907,0.1270401246,-0.02733962
55\C,1.4432161479,-1.3228851071,0.0053702336\H,1.0708281244,-1.8303899
84,0.9044594586\H,1.1010904519,-1.8701964852,-0.8841424199\H,2.5411842
087,-1.3435626354,0.0231370472\C,1.4431286164,0.8803088472,-1.26685115
36\H,1.070484312,1.9125818015,-1.2567392182\H,2.5410827765,0.906140042
9,-1.2759073344\H,1.1009274265,0.3834172996,-2.185440457\C,-0.60908134
99,0.1558470499,0.0224484994\H,-0.972635075,-0.3593235253,0.9198170261
\H,-0.9726052112,1.1905638472,0.0253781155\H,-0.9896401021,-0.35918546
13,-0.8699459352\O,1.3040011033,0.7955203052,1.1300750035\Version=ES6
4L-G09RevE.01\HF=-232.876692\S2=0.752922\S2-1=0.\S2A=0.750006\RMSD=8.3
37e-09\RMSF=2.957e-05\Dipole=-0.3325403,-0.4159532,-0.720158\Quadrupol
e=0.684248,0.1934727,-0.8777208,-1.2548273,-2.0169146,-1.3167036\PG=C0
1 [X(C4H9O1)]\@

HOO*

1\1\GINC-R2418\FOpt\UM11\6-31+G(d,p)\H1O2(2)\ROOT\21-May-2016\0\#\# m11/
6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosy
mm int=ultrafine\HOO*\0,2\O,-1.2306158564,-0.7036090471,0.\H,-1.5271
110676,0.2260132286,0.\O,0.080580664,-0.6700998716,0.\Version=ES64L-G
09RevE.01\HF=-150.8565998\S2=0.752816\S2-1=0.\S2A=0.750005\RMSD=2.773e
-09\RMSF=8.469e-05\Dipole=-0.6032346,0.7408704,0.\Quadrupole=1.3376441
, -1.162277,-0.1753671,-1.5625273,0.,0.\PG=CS [SG(H1O2)]\@

tBuOO*

```
1\1\GINC-R217\FOpt\UM11\6-31+G(d,p)\C4H9O2(2)\ROOT\21-May-2016\0\#\# m1
1/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm
int=ultrafine\|tBuOO*\|0,2\C,0.8872531166,0.1168909583,-0.07646168
44\C,1.4465004482,-1.2949488846,0.0218043514\H,1.0874984793,-1.7900742
456,0.9335770992\H,1.1209316636,-1.8817164725,-0.8472515534\H,2.544052
1348,-1.27533573,0.0403242735\C,1.4315950825,0.8779183203,-1.27848903\
H,1.0687067811,1.9130027665,-1.2684213715\H,2.529707523,0.8842118073,-
1.2656870705\H,1.0939703494,0.3924470958,-2.2040050736\C,-0.6344230276
,0.1474182367,-0.013512755\H,-0.9930429186,-0.3624227783,0.8906561921\
H,-0.9933045106,1.1839068092,-0.0047336411\H,-1.0486055962,-0.36406537
07,-0.8927647446\O,1.4058770788,0.7707713355,1.1480575799\O,1.02932255
57,2.0095338121,1.2492556278\|Version=ES64L-G09RevE.01\HF=-308.0229008
\S2=0.752953\S2-1=0.\S2A=0.750005\RMSD=2.395e-09\RMSF=2.242e-05\Dipole
=-0.244355,-0.8473799,-0.8885811\Quadrupole=1.2912754,-1.0561577,-0.23
51176,-1.8830886,-2.4254581,-2.6141462\PG=C01 [X(C4H9O2)]\|@
```

HO*

```
1\1\GINC-R2886\FOpt\UM11\6-31+G(d,p)\H1O1(2)\ROOT\21-May-2016\0\#\# m11
/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm
int=ultrafine\|HO*\|0,2\O,-1.2226999549,-0.6922980131,0.\H,-1.54888
24151,0.2288128331,0.\|Version=ES64L-G09RevE.01\HF=-75.7068908\S2=0.75
1333\S2-1=0.\S2A=0.750001\RMSD=7.912e-09\RMSF=1.191e-05\Dipole=-0.2541
351,0.7176464,0.\Quadrupole=0.6384776,-0.8707415,0.2322639,-1.9504136,
0.0000001,0.\PG=C*V [C*(H1O1)]\|@
```

int-3

```
1\1\GINC-R222\FOpt\RM11\6-31+G(d,p)\C4H10O3\ROOT\17-May-2016\0\#\# m11/
6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm
m\|Intm 2 'oxonium' - Me3C-O+(O-)OH\|0,1\C,-1.7304395586,-0.7528888842
,-0.2754857629\H,-2.70151719,-0.294201434,-0.5053056065\C,-0.646763144
2,0.2883578616,-0.4971523851\H,-1.5820495337,-1.6133654211,-0.94097427
96\O,0.7629892192,-0.9940002458,0.9939223967\O,0.646008444,-0.52884346
39,-0.2876660963\O,1.7687295611,0.3978818038,-0.5097326004\H,2.2115727
913,0.2022538929,0.3422325448\H,-1.7199852479,-1.0981569401,0.76371330
9\C,-0.6715143159,1.4051847135,0.5239509268\H,0.0952335187,2.158139383
3,0.3073885234\H,-1.6590558847,1.8842880616,0.4835849348\H,-0.51420755
23,0.9901745633,1.5264778634\C,-0.5657824687,0.758756134,-1.9381320138
\H,-1.5157596224,1.2462624298,-2.1953108533\H,0.2485281257,1.478746258
2,-2.0756205085\H,-0.4173474116,-0.0919727929,-2.6161979326\|Version=E
S64L-G09RevE.01\HF=-383.7228295\RMSD=2.386e-09\RMSF=2.240e-05\Dipole=-
0.8223154,0.93678,-0.6334768\Quadrupole=2.4885633,-1.6643914,-0.824171
9,1.2260597,1.4366646,1.7812288\PG=C01 [X(C4H10O3)]\|@
```

TS2b

```
1\1\GINC-R2437\FTS\RM11\6-31+G(d,p)\C4H10O3\ROOT\17-May-2016\0\#\# m11/
6-31+g(d,p) opt=(ts,calcfc,noeigen,cartesian,maxcyc=200) scf=(tight,ma
xcyc=200) freq=noraman nosymm\|TS for int2oxo-zw HOOO* H abstr. formin
g isobutene\|0,1\C,-1.737129969,-0.8960800478,0.3473118581\H,-2.785445
8746,-0.8691044847,0.0118070693\C,-0.8997249028,-0.1220695431,-0.62839
18082\H,-1.4168214718,-1.9433401344,0.406691717\O,0.9859657994,0.58226
60142,1.1714715742\O,0.8338724318,-0.5092996623,0.4146295063\O,1.86123
23713,-0.461611265,-0.6209795724\H,2.5663368758,-0.0385204727,-0.09918
71292\H,-1.68070689,-0.440660168,1.3445528918\C,-0.8534456114,1.297549
4646,-0.4993377858\H,-0.5610706055,1.8530127411,-1.3944995574\H,-1.691
0319696,1.7414597244,0.0495576914\H,0.0473119344,1.3490200049,0.323760
4896\C,-0.538979351,-0.8042135565,-1.9105366698\H,-1.4617331313,-0.894
4170535,-2.5066510555\H,0.1959426308,-0.227152518,-2.4813078866\H,-0.1
473243566,-1.8134062728,-1.7297895527\|Version=ES64L-G09RevE.01\HF=-38
3.7001812\RMSD=5.019e-09\RMSF=3.238e-05\Dipole=-0.9021153,-0.1500405,-
0.8313383\Quadrupole=3.0252109,-0.6585621,-2.3666489,1.0064995,-0.4773
477,-0.6882469\PG=C01 [X(C4H10O3)]\|@
```

alkene

```
1\1\GINC-R2868\FOpt\RM11\6-31+G(d,p)\C4H8\ROOT\21-May-2016\0\#\# m11/6-
31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm
int=ultrafine\|iso-butene\|0,1\C,-0.0168200271,-1.0542326423,-0.014534
006\C,0.6512942923,0.0879653758,-0.1902351097\H,0.128206146,1.03577770
```

61,-0.3316745036\H,1.7427809802,0.1118675107,-0.1981879302\C,-1.523750
4473,-1.1113169238,-0.0001584913\H,-1.8928388799,-1.78181212,-0.791089
8532\H,-1.8861949268,-1.5157203621,0.9571535869\H,-1.9693545786,-0.120
1708412,-0.1494101664\C,0.6843650324,-2.3746873251,0.1829748785\H,0.39
91480876,-2.8235255762,1.1465877537\H,0.3919672683,-3.0889758016,-0.60
16554532\H,1.775321113,-2.2626278602,0.1614765845\Version=ES64L-G09Re
vE.01\HF=-157.1188564\RMSD=7.866e-09\RMSF=7.513e-06\Dipole=-0.1138533,
-0.1946208,0.0299826\Quadrupole=0.4641633,1.0378638,-1.5020271,0.10027
15,0.0145431,-0.3272922\PG=C01 [X(C4H8)]\@

HOOOH

1\1\GINC-R1091\FOpt\RM11\6-31+G(d,p)\H2O3\ROOT\20-May-2016\0\# m11/6-
31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman nosymm
int=ultrafine\HOOOH\0,1\O,0.3313655758,1.0174316541,-0.521925415\H,-
0.2590767667,1.0759782386,0.2476526669\O,1.6078224889,1.0746270178,0.0
579195284\O,1.912720237,-0.2180830594,0.5103827388\H,2.2263079149,-0.6
61412231,-0.2954774391\Version=ES64L-G09RevE.01\HF=-226.6199243\RMSD=
7.184e-09\RMSF=1.565e-05\Dipole=-0.2534487,-0.3522719,-0.0332152\Quad
rupole=1.1728083,-0.1295075,-1.0433008,-2.9177172,-2.665864,1.8674956\P
G=C01 [X(H2O3)]\@

TS3

1\1\GINC-R81\FTS\UM11\6-31+G(d,p)\C4H9O1(2)\ROOT\31-May-2016\0\# m11/
6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) int=ultrafine scf=(tigh
t,maxcyc=300) freq=noraman\BuO beta scission\0,2\C,-0.680636591,1.7
664339963,-0.2383086566\H,-1.3869975106,2.1388382144,0.5039136324\C,-0
.9269493918,-0.3223422968,-0.0210696315\H,0.3786640626,1.8549504236,-0
.0050789563\O,-0.1009412002,-0.6698745594,-0.8867588462\H,-0.954173220
4,1.8790389382,-1.2856130406\C,-2.4203420626,-0.3901032481,-0.33765957
22\H,-2.7444136258,-1.4311023582,-0.1886830833\H,-3.019676329,0.251152
7315,0.321043858\H,-2.5930047622,-0.1254505449,-1.3868833729\C,-0.5533
191437,-0.423495747,1.4571762735\H,-1.1760657255,0.2180597377,2.093488
8741\H,-0.7086400172,-1.4675437743,1.7681961654\H,0.5065715173,-0.1807
315129,1.5929113562\Version=ES64L-G09RevE.01\State=2-A\HF=-232.850482
6\S2=0.769086\S2-1=0.\S2A=0.750065\RMSD=6.214e-09\RMSF=9.823e-07\Dipol
e=-0.7568834,0.6662461,0.7997485\Quadrupole=-0.4265484,1.0615804,-0.63
50319,1.6254588,1.8726433,-1.6961062\PG=C01 [X(C4H9O1)]\@

TS4b

1\1\GINC-R173\FTS\UM11\6-31+G(d,p)\C4H10O3(3)\ROOT\31-May-2016\0\# um
11/6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=20
0) freq=noraman int=ultrafine\TS for H tranfer HOO* to CO*: cage3b (t
riplet)\0,3\C,-0.0946226811,-0.2381215032,0.4406032563\H,0.2281889326
, -0.3986441047,1.4779930246\C,1.1689345047,0.1249070967,-0.3957356275\
H,-0.8206571955,0.5822924406,0.40424856\O,0.6482543635,0.2615789656,-1
.677983046\O,1.5367054252,2.9160057724,-2.7464993121\O,1.928563488,1.7
484291213,-3.1006932804\H,1.3282008394,1.063829741,-2.5374664404\H,-0.
5555370032,-1.154135499,0.0531417586\C,2.1732005627,-1.0342901004,-0.3
525670609\H,3.0412962638,-0.8024034484,-0.9847600237\H,2.525607391,-1.
1944699831,0.6755393605\H,1.7052530442,-1.9556426368,-0.7215788777\C,1
.7736155065,1.4383720951,0.1108319066\H,2.0450639876,1.34398151,1.1709
394932\H,2.6809633038,1.6895956074,-0.4559621444\H,1.0553872666,2.2602
929254,-0.0073425467\Version=ES64L-G09RevE.01\State=3-A\HF=-383.74150
01\S2=2.009733\S2-1=0.\S2A=2.000047\RMSD=9.603e-09\RMSF=2.159e-06\Dipo
le=-0.0127962,-0.8821143,1.3015437\Quadrupole=1.3550265,-1.3746072,0.0
195807,-0.66483,-0.0223413,1.6077575\PG=C01 [X(C4H10O3)]\@

TS4c

1\1\GINC-R2399\FTS\UM11\6-31+G(d,p)\C8H19O1(2)\ROOT\22-May-2016\0\# u
m11/6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) scf=maxcyc=200 freq
=noraman int=ultrafine\BuO* H abstraction from isobutane\0,2\C,-1.4
314361974,-0.0354432957,-0.0136969142\O,-0.3689516778,-0.931387789,-0.
2538323048\C,-2.6894534243,-0.8767522504,-0.3002282132\C,-1.4269518741
,0.4274617101,1.4479826693\C,-1.358735888,1.1595454706,-0.9703676345\H
, -3.5857123079,-0.2561024168,-0.159588434\H,-2.6696920262,-1.246909735
9,-1.3332832103\H,-2.735025599,-1.7347320877,0.3825986049\H,-0.5509253
158,1.0634407553,1.6437307807\H,-2.3300322791,1.0110099185,1.676702052
5\H,-1.3828838366,-0.4429379568,2.1169878078\H,-2.2202616442,1.8285365

195,-0.8316353537\H,-0.4416323309,1.7374773684,-0.7858406717\H,-1.3445
763141,0.8075219766,-2.0104600138\H,0.8152149052,-0.2948473841,0.11111
40265\C,1.948195368,-0.0501885498,0.4315134462\C,2.7546580645,-0.91026
03853,-0.5303448097\C,2.2054463112,1.43943694,0.2581104022\H,3.8312808
333,-0.8265167987,-0.3065161211\H,2.5962739864,-0.5971240699,-1.571311
7639\H,2.4671064978,-1.966933204,-0.4431432613\H,2.0641954202,1.754150
8629,-0.7854335454\H,3.2461949377,1.6719297188,0.5394895798\H,1.547571
0105,2.0454111914,0.8986587389\C,2.0677552925,-0.5168726231,1.87517137
16\H,1.4713948811,0.1074777042,2.5552683162\H,1.7319105286,-1.55798330
65,1.9785132487\H,3.1190726783,-0.4624082826,2.203841206\Version=ES64
L-G09RevE.01\State=2-A\HF=-391.2159024\S2=0.757408\S2-1=0.\S2A=0.75002
3\RMSD=6.932e-09\RMSF=6.771e-07\Dipole=-0.0421196,0.5099011,0.226712\Q
uadrupole=2.870811,-1.938324,-0.932487,-0.3672687,0.1674941,-0.679903\
PG=C01 [X(C8H1901)]\@

CH₃COCH₃

1\1\GINC-R86\FTS\RM11\6-31+G(d,p)\C3H6O1\ROOT\31-May-2016\0\#\# m11/6-3
1+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) int=ultrafine scf=(tight,m
axcyc=300) freq=noraman\acetone\0,1\C,-0.9416881546,-0.3466152506,-0
.0195093833\O,-0.1141931248,-0.1468435907,-0.8855362239\C,-2.417003753
2,-0.4716959149,-0.3422172118\H,-2.7910313811,-1.4517130265,-0.0136926
136\H,-2.9869456132,0.2926614937,0.204731657\H,-2.5736106632,-0.354575
4595,-1.4187747768\C,-0.5508712155,-0.4833554458,1.4381946392\H,-1.063
3353506,0.2825515392,2.0373746629\H,-0.8703181029,-1.4625394279,1.8221
102138\H,0.5328794697,-0.3765139469,1.5444359848\Version=ES64L-G09Rev
E.01\State=1-A\HF=-193.055583\RMSD=8.129e-09\RMSF=7.755e-06\Dipole=-0.
8901791,-0.2149193,0.9316303\Quadrupole=-0.3914899,0.979184,-0.5876942
, -0.4303203,2.1467833,0.4472404\PG=C01 [X(C3H6O1)]\@

CH₃*

1\1\GINC-R197\FOpt\UM11\6-31+G(d,p)\C1H3(2)\ROOT\02-Jun-2016\0\#\# m11/
6-31+g(d,p) opt=(maxcyc=200) int=ultrafine scf=(tight,maxcyc=300) freq
=noraman\H3C*\0,2\C,0.0818016349,-0.72932329,0.\H,-1.0035918008,-0.7
2932329,0.\H,0.624472363,0.2106751276,0.\H,0.624472363,-1.6693217076,0
.\Version=ES64L-G09RevE.01\State=2-B\HF=-39.8057247\S2=0.752387\S2-1
=0.\S2A=0.750004\RMSD=1.326e-09\RMSF=1.043e-05\Dipole=-0.0000038,0.,0.
\Quadrupole=0.5341657,0.5343526,-1.0685184,0.,0.,0.\PG=C02V [C2(H1C1),
SGV(H2)]\@

CH₃OO*

1\1\GINC-R197\FOpt\UM11\6-31+G(d,p)\C1H3O2(2)\ROOT\02-Jun-2016\0\#\# m1
1/6-31+g(d,p) opt=(maxcyc=200) int=ultrafine scf=(tight,maxcyc=300) fr
eq=noraman\H3COO*\0,2\C,-0.0110216407,0.8289442451,-0.018832786\H,0.
3858133426,-0.1891471241,0.0414259257\H,0.3659936909,1.3519527463,-0.9
052622568\H,-1.1070086232,0.8311899384,-0.0032395114\O,0.4694611198,1.
5075397579,1.1575671753\O,0.0537709921,2.7402834616,1.1904427903\Ver
sion=ES64L-G09RevE.01\State=2-A\HF=-190.1391272\S2=0.752888\S2-1=0.\S2
A=0.750005\RMSD=8.768e-09\RMSF=5.068e-05\Dipole=-0.1738726,-0.873713,-
0.7883526\Quadrupole=0.1500093,-0.1913626,0.0413532,0.3664319,-0.34840
64,0.203333\PG=CS [SG(C1H1O2),X(H2)]\@

CH₃OOH

1\1\GINC-R216\FOpt\UM11\6-31+G(d,p)\C1H4O2\ROOT\03-Jun-2016\0\#\# um11/
6-31+g(d,p) opt=(maxcyc=200) int=ultrafine scf=(tight,maxcyc=300) freq
=noraman\H3COOH\0,1\C,-0.9667720845,-0.4609032749,-0.0000170784\H,-1
.9557592454,0.011876045,-0.0000216217\H,-0.8374599743,-1.0774108381,0.
9017740966\H,-0.8373786264,-1.0773613046,-0.9018272875\O,-0.0474281285
,0.6128558428,0.0000706861\O,1.2403895494,-0.0133160199,0.0002071519\H
,1.8142844797,0.7660033298,-0.001940667\Version=ES64L-G09RevE.01\Stat
e=1-A\HF=-190.7800077\S2=0.\S2-1=0.\S2A=0.\RMSD=3.576e-09\RMSF=4.444e-
05\Dipole=-0.1322535,0.0338437,-0.0016635\Quadrupole=2.415525,-0.86834
92,-1.5471758,2.6820703,-0.0063029,-0.0030975\PG=C01 [X(C1H4O2)]\@

int-1w

1\1\GINC-R227\FOpt\UM11\6-31+G(d,p)\C4H12O4\ROOT\26-Jun-2016\0\#\# um11/
6-31+g(d,p) opt=(maxcyc=200) int=ultrafine scf=(tight,maxcyc=300) fre
q=noraman # guess=read geom=allcheck\i-Butane + H2O + O3 complex\0,1
\C,1.1005493273,-1.493096178,0.7539285861\H,1.6224501583,-2.2962279135


```
,0.2095398806\C,1.4863060982,-0.1270271979,0.1782915561\H,1.370967291,
-1.5746833679,1.8166701945\O,-0.8002230773,2.3576681918,0.0531563518\O
,-1.5311087,1.3371167355,0.027661434\O,-1.5556744337,0.648654199,1.082
5960364\H,0.9711581655,0.6519374573,0.7666087652\H,0.0198356715,-1.670
0619826,0.6516656885\C,1.0384332163,-0.0209375377,-1.283719721\H,1.598
0236973,-0.7437341231,-1.8987742846\H,-0.0309263777,-0.2546865779,-1.3
976415396\H,1.2293037499,0.9831063512,-1.6914169428\C,2.9934513987,0.1
143116946,0.3055519105\H,3.2763572888,1.0992702764,-0.0927949353\H,3.3
215031003,0.0628854655,1.3537658897\H,3.550562851,-0.6496330796,-0.259
5913922\H,-2.5541305008,-1.2583236671,0.0276863979\O,-2.2706304445,-1.
2556473695,-0.8936135425\H,-2.65869848,-2.0266193765,-1.318649333\Ver
sion=ES64L-G09RevE.01\State=1-A\HF=-460.0961423\S2=0.346492\S2-1=0.\S2
A=0.002586\RMSD=6.137e-09\RMSF=4.845e-06\Dipole=-0.7177686,-0.6115562,
0.1010509\Quadrupole=2.3605968,0.5545603,-2.9151571,3.74491,-0.4378486
,0.9455786\PG=C01 [X(C4H12O4)]\@
```

TS1aw

```
1\1\GINC-R122\FTS\UM11\6-31+G(d,p)\C4H12O4\ROOT\28-Jun-2016\0\#\# um11/
6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200)
freq=noraman int=ultrafine # guess=read geom=allcheck\TS for O3---H2O
tertiary H abstraction\0,1\C,0.8957862136,0.9667750985,-1.2769285743
\H,1.5267569641,1.8650687973,-1.3884792651\C,1.3360804122,0.2086204025
,-0.0355422686\H,1.0127673074,0.359513639,-2.184652664\O,-0.1810292922
,-1.871472632,0.2260185777\O,-1.355802991,-1.2740004632,0.403546322\O,
-1.9130057125,-0.9368191315,-0.6941478945\H,0.6884419632,-0.8214582293
,-0.0337255813\H,-0.1478013098,1.2965975024,-1.1895387975\C,0.92832745
51,0.8781720258,1.2632517703\H,1.4579834761,1.8413794785,1.3555403989\
H,-0.1492309784,1.0960517923,1.2764577166\H,1.1921966044,0.2609980129,
2.1331053586\C,2.7777868068,-0.2686476405,-0.0735683454\H,3.0154206413
,-0.9045044119,0.7898383462\H,2.9948943213,-0.8258061251,-0.9947770393
\H,3.4492597953,0.6056223,-0.0429416881\H,-2.6071059383,0.9239820517,-
0.1545849994\O,-2.212163172,1.7376931445,0.1870898646\H,-2.9213115665,
2.3734043878,0.3207337625\Version=ES64L-G09RevE.01\State=1-A\HF=-460.
0764921\S2=0.714073\S2-1=0.\S2A=0.033169\RMSD=9.882e-09\RMSF=1.630e-06
\Dipole=0.1303113,0.611448,0.0777964\Quadrupole=5.2522849,-2.4489363,-
2.8033486,-2.8975518,-0.6975507,-0.1133551\PG=C01 [X(C4H12O4)]\@
```

Polymers

Poly(propylene)

pProp

```
1\1\GINC-R153\FOpt\RM11\6-31+G(d,p)\C7H16\ROOT\03-Apr-2016\0\#\# opt=ma
xcyc=200 freq=noraman 6-31+g(d,p) nosymm scf=(tight,maxcyc=200) m11\p
oly-Propylene\0,1\C,1.1990116359,0.3854088171,0.3009965964\C,-0.10852
30132,-0.378981976,0.5592630503\H,0.136371375,-1.3155175464,1.09271501
67\H,-0.7350058226,0.2133758163,1.2508460993\C,-0.9503008132,-0.723170
8676,-0.6794473101\C,2.0968008473,-0.34690427,-0.7020096464\H,3.062758
6714,0.1660608095,-0.813194189\H,1.6359763444,-0.413302602,-1.69780908
39\H,2.2992794449,-1.3733241201,-0.3558197095\C,-2.2407451615,-1.42983
39407,-0.251028947\H,-2.0270975792,-2.324437557,0.351630164\H,-2.83648
59312,-1.7392219471,-1.1216536655\H,-2.8622380829,-0.7549406982,0.3583
487136\H,-0.3739118399,-1.4210401639,-1.3098873194\H,0.9475045298,1.37
5703823,-0.1149486792\C,1.9425346188,0.6017366326,1.6234416462\H,1.312
0871712,1.1254888404,2.3565862485\H,2.2326598101,-0.3663726999,2.06149
16092\H,2.8585554501,1.1917753534,1.4773070873\C,-1.2766035094,0.52300
24625,-1.5097740828\H,-1.7771616111,1.2793919065,-0.8838071246\H,-0.37
51072327,0.9845530131,-1.9368772752\H,-1.951899412,0.2764567743,-2.341
5663189\Version=ES64L-G09RevE.01\HF=-276.2133336\RMSD=3.310e-09\RMSF=
1.385e-05\Dipole=0.0109355,0.0098152,-0.034891\Quadrupole=-0.2354155,0
.3361715,-0.100756,0.0111638,-0.0315231,0.1512625\PG=C01 [X(C7H16)]\@
```

int-1

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1\1\GINC-R408\FOpt\UM11\6-31+G(d,p)\C7H16O3\ROOT\03-May-2016\0\#\# um11
/6-31+g(d,p) int=ultrafine opt=(maxcyc=200) scf=(tight,maxcyc=200) nos
ymm freq=noraman # guess=read geom=allcheck iop(1/8=1)\O3 + pPropylen
e caged complex\0,1\C,1.0170120052,0.8979938281,0.8473610848\C,0.5730
912458,0.2218007064,-0.4593304874\H,-0.527404372,0.2911652296,-0.54676
```

32822\H,0.9723331303,0.8109191663,-1.3047988423\C,0.9972062011,-1.2438
668253,-0.6485332672\C,0.614735882,2.3768287598,0.8301890485\H,0.84419
83553,2.8655627871,1.7876694554\H,-0.459273311,2.5008646352,0.63090086
18\H,1.1654348427,2.9102222155,0.0394827729\C,0.5961760999,-2.13320653
83,0.533699121\H,1.0363038536,-1.7931150767,1.4817163819\H,0.921314726
, -3.170086197,0.3671099592\H,-0.4981693298,-2.1509543045,0.6512890174\
O,-2.3343332899,-0.3600016337,1.372589132\O,-2.2733767443,0.8962109883
,1.4538126275\O,-2.7156395023,-0.8269646773,0.2646627428\H,2.095926181
9,-1.2717193528,-0.7420850567\H,0.4971237022,0.4107084475,1.6912038613
\C,0.39378537,-1.7915487646,-1.9462819417\H,-0.7061839065,-1.798552609
5,-1.8786809816\H,0.6730596736,-1.1731915629,-2.8114964694\H,0.7250890
775,-2.8215891614,-2.1405780501\C,2.5274869233,0.7650218791,1.07153357
57\H,2.839352201,-0.2807638387,1.2014960892\H,3.0774250618,1.174916555
8,0.209121921\H,2.8420549227,1.3228703442,1.9649897262\\Version=ES64L-
G09RevE.01\HF=-501.5521161\S2=0.393404\S2-1=0.\S2A=0.003499\RMSD=7.398
e-09\RMSF=1.099e-05\Dipole=0.1094162,-0.1309022,0.1744526\Quadrupole=0
.3694201,-0.7814839,0.4120638,0.3194108,-1.437653,-0.5169385\PG=C01 [X
(C7H16O3)]\@

TS1a

1\1\GINC-R155\FTS\UM11\6-31+G(d,p)\C7H16O3\ROOT\03-Apr-2016\0\#\ um11/
6-31+g(d,p) int=ultrafine opt=(ts,calcf, noeigen,maxcyc=200) scf=(tigh
t,maxcyc=200) nosymm freq=noraman # guess=read geom=allcheck\TS for O
3 H abstraction of pPropylene (pos. b)\0,1\C,1.7787191818,-0.84954819
8,0.1454916533\C,0.6382498857,-0.6007828446,1.1432967101\C,1.258979164
5,-1.3533820862,-1.2055320431\C,-0.4237958597,0.4130738253,0.732953596
8\H,1.0698004707,-0.2414021026,2.0974948447\H,2.0952312618,-1.61584093
78,-1.8686499949\H,0.6390431374,-2.2533987352,-1.0692569214\H,0.640725
7795,-0.6080781971,-1.7243701119\C,-1.4736462906,0.6502586412,1.805257
5692\H,-2.3087628303,1.2457234673,1.4134136586\H,-1.8707969168,-0.2977
770154,2.192670638\H,-1.0220188793,1.1991628542,2.6484588454\H,0.14734
79255,-1.5614450906,1.3784182626\O,-1.9252112425,-0.5358183199,-1.1324
322497\O,-1.9984474147,0.5359033213,-1.94412875\O,-2.7244447217,1.4664
879414,-1.4665081668\H,-1.0753374358,-0.1367614595,-0.1633310612\H,2.3
117970972,0.1025814079,-0.0156175389\C,0.1120576956,1.6903175796,0.107
7343738\H,0.8677477596,2.1342057409,0.7780383588\H,0.6003118836,1.5087
174001,-0.8605965558\H,-0.6893283237,2.4246829807,-0.0424906029\C,2.77
11350758,-1.8530363806,0.7431712374\H,3.1637218429,-1.5060319167,1.709
83566\H,2.2810372608,-2.8253197887,0.9073975166\H,3.6228668527,-2.0177
11977,0.0687660013\\Version=ES64L-G09RevE.01\HF=-501.5300418\S2=0.7685
3\S2-1=0.\S2A=0.041952\RMSD=6.472e-09\RMSF=1.183e-05\Dipole=0.9320637,
-0.0237589,0.7562663\Quadrupole=-2.3074447,0.9986218,1.3088229,1.30308
58,-2.6924813,0.9952062\PG=C01 [X(C7H16O3)]\@

TS1b

1\1\GINC-R154\FTS\UM11\6-31+G(d,p)\C7H16O3\ROOT\03-Apr-2016\0\#\ um11/
6-31+g(d,p) int=ultrafine opt=(ts,calcf, noeigen,maxcyc=200) scf=(tigh
t,maxcyc=200) nosymm freq=noraman # guess=read geom=allcheck\TS for O
3 H abstraction of pPropylene (pos. a)\0,1\C,0.838629367,-1.190127556
8,0.6926470912\C,0.408935519,0.2594243714,0.5075515481\C,0.8282386236,
-1.9999362669,-0.6085780071\C,0.9093928555,1.0424969602,-0.6962968119\
H,0.5104025917,0.8369384199,1.4431765808\H,1.1081140409,-3.0429105754,
-0.4063618594\H,-0.1714054985,-2.00337569,-1.0666783453\H,1.5353095382
, -1.6012811314,-1.3489327345\C,0.2307547178,2.4134113448,-0.7738125674
\H,0.6016604039,2.9826114976,-1.6371773798\H,-0.8578904952,2.307284248
3,-0.8724943475\H,0.4417475074,3.0012236369,0.1332740027\H,-0.84024982
58,0.2558785654,0.4215509886\O,-2.1629456043,0.2611023824,0.3237669164
\O,-2.4068016519,-0.6866895694,-0.6082459546\O,-2.0161512177,-0.340001
1074,-1.7686663377\H,0.6581880196,0.479143409,-1.6080383428\H,1.881579
8339,-1.1483623479,1.0608563078\C,-0.0107877991,-1.8709151745,1.774192
1165\H,-0.0284892001,-1.2798638744,2.7008824922\H,-1.0491313832,-1.988
4285292,1.4306069305\H,0.3834763997,-2.8685659137,2.0099706045\C,2.438
5833791,1.1915705395,-0.6095414888\H,2.7217792447,1.7227427647,0.31229
94219\H,2.9479261816,0.2175797296,-0.6120602506\H,2.813411732,1.774103
0772,-1.4625685137\\Version=ES64L-G09RevE.01\HF=-501.5272227\S2=0.7830
74\S2-1=0.\S2A=0.045124\RMSD=6.630e-09\RMSF=3.582e-06\Dipole=1.0679669
, -0.0316101,0.4228774\Quadrupole=-1.7193047,1.8759384,-0.1566336,0.153
3276,-0.9796533,-0.8046329\PG=C01 [X(C7H16O3)]\@

int-2 (rad)

```
1\1\GINC-R823\FOpt\UM11\6-31+G(d,p)\C7H15(2)\ROOT\10-Jun-2016\0\#\ um1
l/6-31+g(d,p) opt=maxcyc=200 scf=(tight,maxcyc=200) freq=noraman int=u
ltrafine\pPropylene-C* (tertiary)\0,2\C,1.913206028,-1.2188300554,0.
0851928402\H,3.0195853649,-1.1528601647,0.0961349053\C,1.2865355363,0.
090325047,0.4545536034\H,1.6424725611,-2.0252242673,0.7831719401\H,1.6
174300632,-1.5319872478,-0.9254454131\C,1.0184498789,1.0782913053,-0.6
368581082\C,1.476628181,0.6216744202,1.8459198984\H,1.9475084683,1.592
6451443,-0.9549516157\H,0.603314202,0.5920958522,-1.5315251277\H,0.318
1688785,1.860816013,-0.3106888016\H,2.4936006963,1.0634332886,1.930163
2243\H,0.7776929381,1.4607618124,2.0136926475\C,1.2978834251,-0.396847
8191,2.9848164788\H,2.0280963046,-1.2107949553,2.8410343195\C,-0.11268
78358,-0.993193403,2.9670889108\C,1.5861583628,0.2649424983,4.33568121
37\H,-0.3345727889,-1.4818127569,2.0079299766\H,-0.2443068184,-1.73116
34086,3.7713331638\H,-0.8600091747,-0.1974075842,3.1141973515\H,1.4843
027346,-0.453138544,5.161719143\H,2.6025003009,0.6830578841,4.37036036
68\H,0.8772096933,1.087872941,4.5179530824\Version=ES64L-G09RevE.01\St
ate=2-A\HF=-275.5529854\S2=0.753438\S2-1=0.\S2A=0.75001\RMSD=9.736e-0
9\RMSF=1.852e-06\Dipole=0.1366617,0.0075775,-0.0323101\Quadrupole=-0.3
201022,0.1480716,0.1720306,-0.3493506,-0.1673731,-0.1507144\PG=C01 [X(
C7H15)]\@\
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hydrotrioxide

```
1\1\GINC-R168\FOpt\RM11\6-31+G(d,p)\C7H16O3\ROOT\03-Apr-2016\0\#\ opt=
maxcyc=200 freq=noraman ml/6-31+g(d,p) int=ultrafine scf=maxcyc=200\
Intm 2 'zwitterionic' - OOH pos. b\0,1\C,1.6597947446,-0.3606680572,-
0.1407279841\C,0.529859628,-0.3476539921,0.9007502509\C,1.219274717,-0
.9331027326,-1.4940918956\C,-0.7224495281,0.4909090175,0.6037277749\H,
0.9376871119,0.0258561085,1.8551082226\H,2.0880332796,-1.0647011449,-2
.155384838\H,0.7456867885,-1.9179375773,-1.3534645438\H,0.489061998,-0
.2916941122,-2.0018367515\C,-1.6219944743,0.548877112,1.8378921611\H,-
2.5710896863,1.0438076567,1.5951332631\H,-1.8431229201,-0.4605697809,2
.2089426798\H,-1.1161189914,1.1129904642,2.6338632094\H,0.2029171898,-
1.3835552068,1.0912276705\O,-3.1920911853,-1.3325278762,0.2345988676\O
,-1.8602871049,-1.3847807922,-0.2247138365\O,-1.4668205958,-0.07179930
45,-0.5189160527\H,-3.6968267954,-1.3203937376,-0.5946554916\H,2.01201
87587,0.6738686969,-0.2916533685\C,-0.3910287323,1.8908183709,0.094601
2973\H,0.2654222243,2.398100203,0.8151400548\H,0.1214910083,1.84449850
72,-0.8751839851\H,-1.309589615,2.480392176,-0.0230422753\C,2.83310154
97,-1.1776252196,0.4153532727\H,3.1808430206,-0.7826116639,1.380935704
3\H,2.5303538245,-2.2251834831,0.5692087791\H,3.6832828754,-1.17422380
18,-0.2811834553\Version=ES64L-G09RevE.01\State=1-A\HF=-501.6462343\R
MSD=5.988e-09\RMSF=3.256e-06\Dipole=0.0103148,0.4521472,0.0101653\Quad
rupole=2.0349552,-1.0113724,-1.0235828,0.423872,2.8289873,1.4832338\PG
=C01 [X(C7H16O3)]\@\
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TS2a

```
1\1\GINC-R1676\FTS\UM11\6-31+G(d,p)\C7H16O3\ROOT\17-Apr-2016\0\#\ um11
/6-31+g(d,p) int=ultrafine opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tig
ht,maxcyc=200) nosymm freq=noraman # guess=read geom=allcheck\TS for
peroxyl radical addition to *OpPropylene pos. b\0,1\C,-1.76187478
62,-0.0659571438,0.2066268985\C,-0.6956237871,0.6363513456,-0.64925068
55\C,-1.3526353661,-1.4895572291,0.6113666952\C,0.6039707847,1.0992561
037,0.0435127801\H,-1.1426066061,1.5347477126,-1.1074764498\H,-2.18143
2696,-2.0033687112,1.1191371638\H,-1.1057187973,-2.0690292025,-0.29633
38414\H,-0.4863988476,-1.4713285319,1.2848860922\C,1.5714817628,1.6855
854251,-0.9921005609\H,2.5018662373,1.9953144448,-0.4987467546\H,1.816
2795807,0.9297885115,-1.7502810929\H,1.1237703996,2.5553007073,-1.4937
515565\H,-0.4191222335,-0.0320676598,-1.4816341584\O,1.7782115339,-2.4
366141898,0.0893069681\O,1.5965778118,-1.3422578104,-0.6187616096\O,1.
230066305,0.0798518345,0.7685803557\H,0.8807852811,-2.74223847,0.32536
85372\H,-1.9312604673,0.5193510167,1.1252307721\C,0.312160802,2.150249
2888,1.1406073544\H,-0.2282541242,2.992014946,0.6856012423\H,-0.297862
8657,1.7252773923,1.9468076221\H,1.2528909474,2.5179537083,1.568532843
\C,-3.0816089081,-0.1140822011,-0.5746812802\H,-3.4332389103,0.8942043
655,-0.8353431323\H,-2.9500146748,-0.6766881631,-1.5124636488\H,-3.870
905376,-0.6116914901,0.0063854462\Version=ES64L-G09RevE.01\HF=-501.60
35041\S2=0.741173\S2-1=0.\S2A=0.01859\RMSD=5.320e-09\RMSF=6.290e-06\Di
```

pole=-0.987313,0.2034397,-0.0093296\Quadrupole=-4.4372118,4.8719773,-0.4347654,2.5566257,-0.8462871,-0.5629447\PG=C01 [X(C7H16O3)]\@

alkoxyyl

1\1\GINC-R3467\FOpt\UM11\6-31+G(d,p)\C7H15O1(2)\ROOT\20-May-2016\0\#\m11/6-31+g(d,p) opt=(maxcyc=200) freq=noraman nosymm scf=(tight,maxcyc=200) int=ultrafine\pPropylene-O* (tertiary)\0,2\C,1.365868215,0.0073936155,-0.4961567922\C,0.541656756,-0.3387452462,0.7521061815\C,0.5758550676,-0.227071288,-1.7875077556\C,-0.8055472885,0.4048483859,0.8858970038\H,1.1425000351,-0.1276867611,1.6525701965\H,1.2039964966,-0.0328638233,-2.6687248853\H,0.2265659238,-1.2696550944,-1.8382965603\H,-0.3124017443,0.4176998601,-1.8558759141\C,-1.4359440483,0.0446563409,2.2603551233\H,-2.4379499305,0.4826606216,2.3463508281\H,-1.5046302807,-1.044043232,2.3739851756\H,-0.7941510465,0.4560211563,3.0510116729\H,0.3191857358,-1.4190850234,0.7510791907\O,-1.7330478484,-0.091380614,-0.013285415\H,1.6471633645,1.0727222285,-0.4429657169\C,-0.664600131,1.9272623105,0.7580148054\H,0.0919044488,2.3089069771,1.4591532706\H,-0.3635460875,2.2026152109,-0.2613687253\H,-1.6264246699,2.4110422333,0.9725972282\C,2.6561294521,-0.8209534043,-0.5003769771\H,3.2416689357,-0.6612739142,0.416538058\H,2.4211608401,-1.8945069455,-0.5681612524\H,3.2907398043,-0.5622575944,-1.3595567404\Version=ES64L-G09RevE.01\HF=-350.7434519\S2=0.753079\S2-1=0.\S2A=0.750007\RMSD=5.344e-09\RMSF=9.437e-06\Dipole=0.565493,0.2665645,0.5892398\Quadrupole=-2.3935671,0.4315664,1.9620008,-0.4452717,-1.8541212,0.2096957\PG=C01 [X(C7H15O1)]\@

TS3a

1\1\GINC-R121\FTS\UM11\6-31+G(d,p)\C7H15O1(2)\ROOT\20-May-2016\0\#\m11/6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) freq=noraman nosymm scf=(tight,maxcyc=200) int=ultrafine\TS for C-Calpha fragmentation : pPropylene-O* (tertiary)\0,2\C,1.6589115633,-0.139154919,-0.5327063937\C,0.9018964214,-0.5994719184,0.6799183652\C,0.9194922966,-0.4454680523,-1.8382506248\C,-0.9389148343,0.3778089343,0.8863484226\H,1.3166341504,-0.3148892721,1.652290513\H,1.5226018893,-0.1347859858,-2.7030233603\H,0.7355765443,-1.5274880638,-1.9225111851\H,-0.0559053346,0.0541817604,-1.8752508947\C,-1.2147858501,-0.0618709031,2.3254191423\H,-2.1906014687,0.3547049822,2.6155277874\H,-1.2838286873,-1.1547169523,2.3797317812\H,-0.4595775823,0.3060453874,3.0319763195\H,0.4984661359,-1.6155639147,0.6419601717\O,-1.5752073845,-0.1715433408,-0.0401712069\H,1.8299903258,0.9468283097,-0.4538902072\C,-0.4750169357,1.8237480771,0.716376844\H,0.3851879855,2.068174735,1.3542463615\H,-0.235546089,2.0189464653,-0.3355750808\H,-1.3113546464,2.4784559916,1.0044800098\C,3.0421013894,-0.8263212391,-0.5216916345\H,3.6023698808,-0.6039610408,0.3970278818\H,2.9294967488,-1.9176318065,-0.60043133\H,3.6389714812,-0.4855372345,-1.3794866821\Version=ES64L-G09RevE.01\HF=-350.7230908\S2=0.768242\S2-1=0.\S2A=0.750067\RMSD=5.065e-09\RMSF=5.331e-07\Dipole=1.0400132,0.3367775,0.7095997\Quadrupole=-2.3579324,0.8915713,1.4663611,-1.4162627,-1.8720548,0.266526\PG=C01 [X(C7H15O1)]\@

TS4(1,4)

1\1\GINC-R156\FTS\UM11\6-31+G(d,p)\C7H15O1(2)\ROOT\07-Jun-2016\0\#\m11/6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) freq=noraman nosymm scf=(tight,maxcyc=200) int=ultrafine\TS for 1,4 pPropylene-O* (tertiary) H abstraction\0,2\C,1.3036660205,0.0284283781,0.0322398468\C,0.0907751869,0.2204724367,-0.901831958\C,2.2729008501,1.1969060786,0.0425400727\C,-1.1448119267,0.0264425518,0.0094785093\H,0.0933451913,-0.4809473172,-1.7509050513\H,3.0639803526,1.0594626262,0.7925127333\H,2.7561937108,1.2892830476,-0.9448580072\H,1.7501473198,2.1395712741,0.2530342056\C,-2.2714801144,1.0096542291,-0.3125241727\H,-3.1074746484,0.8798590403,0.3880675084\H,-1.9049236241,2.0413629483,-0.2338519986\H,-2.6428986864,0.8377341855,-1.3332738338\H,0.0960532324,1.2415909538,-1.312412916\O,-0.6652917347,0.3432701895,1.3176625252\H,0.6722832049,0.0922311624,1.0796089117\C,-1.6628385123,-1.4147763601,-0.0163904301\H,-2.0335077683,-1.6826710967,-1.0166554597\H,-0.8683747181,-2.1188531767,0.2638095258\H,-2.4823700997,-1.5281425632,0.7061514261\C,1.9922072471,-1.3222992615,-0.0586902746\H,1.2818753109,-2.1564459264,-0.001948616\H,2.5186770077,-1.3979377052,-1.0251110134\H,2.737513198,-1.4465616952,0.7386734665\Version=ES64L-G09RevE.01\HF=-350.7142399\S2=0.757654\S2-1=0.\S2A=0.750022\RMSD=5.660e-09\RMSF=2.519e-06\Dipole=0.3721443,-0.172

6898,-0.8274925\Quadrupole=2.3262309,0.170593,-2.496824,0.1356354,1.397082,-0.7289362\PG=C01 [X(C7H15O1)]\@

TS4(1,5)

1\1\GINC-R148\FTS\UM11\6-31+G(d,p)\C7H15O1(2)\ROOT\07-Jun-2016\0\#\# m1/6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) freq=noraman nosymm scf=(tight,maxcyc=200) int=ultrafine\TS for 1,5 pPropylene-O* (tertiary) H abstraction\0,2\C,1.4122800293,-0.0768580072,0.3238365773\C,0.1971802538,-0.8385532322,-0.2277505024\C,1.4065979135,1.3319000945,-0.2470840496\C,-1.114807136,-0.0521352963,-0.0112175989\H,0.1160301909,-1.8341434043,0.236783699\H,1.8101818116,2.1182149413,0.4012244779\H,1.8167997458,1.3944130127,-1.2638347642\H,0.202486401,1.5839879744,-0.4265310479\C,-2.2732643584,-0.7951354826,-0.6950142067\H,-3.1993253385,-0.2128975871,-0.6039318466\H,-2.0529942932,-0.9405973945,-1.7603075011\H,-2.4227216487,-1.7745159756,-0.2186301632\H,0.3273701811,-0.9844420205,-1.3135406613\O,-1.0185689273,1.1928870578,-0.6703813818\H,1.3203626599,-0.0207085515,1.4193383937\C,-1.4179655713,0.1597656373,1.4774564464\H,-1.4348181981,-0.7954076592,2.0230494309\H,-0.6656256937,0.8151779815,1.9372369387\H,-2.3956168852,0.6472547608,1.5883625641\C,2.7180024493,-0.8139718361,-0.0104379552\H,2.7196929697,-1.8260753845,0.4183463823\H,2.8369458809,-0.9060523916,-1.100415551\H,3.5912385635,-0.2746632371,0.3813313195\Version=ES64L-G09RevE.01\HF=-350.7243347\S2=0.757136\S2-1=0.\S2A=0.750022\RMSD=4.207e-09\RMSF=1.717e-06\Dipole=0.5311021,-0.6127517,0.4020981\Quadrupole=1.0814007,-0.9374791,-0.1439216,2.6428561,-0.902355,1.1764373\PG=C01 [X(C7H15O1)]\@

ROOH

1\1\GINC-R182\FOpt\RM11\6-31+G(d,p)\C4H10O2\ROOT\26-Jun-2016\0\#\# m1/6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=noraman\beta-scission C fragment peroxide\0,1\C,-0.000011544,0.0505658389,-0.3541289244\C,-1.2649991109,-0.6792357063,0.1110523733\H,-1.2927095475,-1.7023184419,-0.2887976646\H,-1.2902871978,-0.7396766137,1.2078077829\H,-2.1739583158,-0.1572148462,-0.220266767\H,-0.0000359467,0.0918271138,-1.4556669052\C,1.265001149,-0.6792278066,0.1109969098\H,2.1739424457,-0.1571993306,-0.2203593439\H,1.2903362786,-0.7396713014,1.2077511114\H,1.292702138,-1.7023092867,-0.2888569468\C,-0.0000059178,1.5057129094,0.1102121396\H,0.8983801751,2.0412548897,-0.2405969908\H,-0.8984152034,2.0412471295,-0.2405495407\O,0.0000319845,1.4960352819,1.5320289368\O,0.0000367741,2.8753244281,1.9130375097\H,0.000062989,2.7908312119,2.8770452698\Version=ES64L-G09RevE.01\State=1-A\HF=-308.6505989\RMSD=2.558e-09\RMSF=6.051e-05\Dipole=0.0000003,-0.2021613,-0.0350069\Quadrupole=-1.4203158,-2.1570663,3.5773821,0.000048,0.000126,1.7042322\PG=C01 [X(C4H10O2)]\@

Poly(styrene)

pSty

1\1\GINC-R47\FOpt\UM11\6-31+G(d,p)\C17H20\ROOT\03-Apr-2016\0\#\# um11/6-31+g(d,p) opt=maxcyc=200 scf=(tight,maxcyc=200) nosymm freq=noraman\poly-styrene\0,1\C,1.7924253906,-1.4648361817,0.6254127652\C,0.5161556703,-2.2605514152,1.0024316108\H,0.8093949685,-3.3032736347,1.2074071231\H,0.1184867685,-1.8616682468,1.9514812966\C,-0.6128013316,-2.3089902224,-0.0451595975\C,1.6365665797,0.0546158098,0.7673459276\H,2.6005152155,0.5557022128,0.5988960543\H,1.2950749154,0.3010371606,1.7829567917\H,0.9038449038,0.4785758394,0.0689703884\C,-1.7096480968,-3.2811196374,0.4178377595\H,-1.3000120819,-4.2914623784,0.5585344164\H,-2.5246908212,-3.3348228155,-0.316223767\H,-2.1418064412,-2.955827456,1.3763437771\H,-0.1830174472,-2.6959256732,-0.9832847895\H,2.5580213458,-1.771732538,1.3579685368\C,-1.2007538787,-0.9403590139,-0.3421760098\C,-1.1580036428,-0.40612695,-1.6317501852\C,-1.788342562,-0.1795690642,0.6746925951\C,-1.661498972,0.8675951224,-1.8969678389\H,-0.7023602474,-0.9928451345,-2.4335505528\C,-2.2924069712,1.0915493945,0.4168093825\H,-1.8364914724,-0.5817517588,1.6902533949\C,-2.2242482755,1.6238571121,-0.8714337117\H,-1.6114731476,1.2706469927,-2.9099753175\H,-2.7377586965,1.6739759255,1.2251896414\H,-2.6134934562,2.6225217415,-1.0743310068\C,2.3058945091,-1.9075885621,-0.7383404629\C,2.8303805435,-3.1989049468,-0.8778839943\C,2.2413383983,-1.0970402048,-1.8733991342\C,3.2668050133,-3.6725693272,-2.1110192791\H,2.8985244034,-3.8426756026,0.0038750

251\C,2.6766478483,-1.5671203592,-3.1140318848\H,1.8410635388,-0.08497
05407,-1.795771568\C,3.1876817733,-2.8556775791,-3.2393607505\H,3.6732
661514,-4.6820527244,-2.1924212093\H,2.6166714049,-0.9159074813,-3.987
9726031\H,3.5285820797,-3.2210397321,-4.2090281437\Version=ES64L-G09R
evE.01\HF=-659.4606258\S2=0.\S2-1=0.\S2A=0.\RMSD=4.396e-09\RMSF=1.097e
-05\Dipole=-0.0087514,-0.0700864,0.1265283\Quadrupole=-5.9883334,2.562
8206,3.4255128,-3.3956017,-1.3250822,-1.1867239\PG=C01 [X(C17H20)]\@

int-1

1\1\GINC-R315\FOpt\UM11\6-31+G(d,p)\C17H20O3\ROOT\05-Apr-2016\0\#\ um1
1/6-31+g(d,p) int=ultrafine opt=(maxcyc=200) scf=(tight,maxcyc=200) no
symm freq=noraman # guess=read geom=allcheck\O3 + pStyrene caged comp
lex\O,1\C,-0.4836785888,0.926739635,-0.3749122819\C,-1.1509680503,-0.
3076568118,-1.0317521393\H,-2.0740577159,0.0307421379,-1.5310676853\H,
-0.4868845222,-0.6930473993,-1.8254030637\C,-1.5637925237,-1.462543764
1,-0.0987624299\C,0.9949644251,0.7194668813,-0.0240915554\H,1.44092784
59,1.6633556768,0.3208033268\H,1.5468515691,0.3867591893,-0.9148622711
\H,1.1509506129,-0.0379373802,0.7545315068\C,-2.3529613432,-2.51313705
33,-0.8953100385\H,-3.2470717483,-2.0631554643,-1.3507548678\H,-2.6715
599898,-3.3420464352,-0.2493905034\H,-1.7376534175,-2.9350955618,-1.70
44652693\O,-2.9612630081,1.2804029289,-3.7391596785\O,-3.9260144219,0.
9723065208,-2.9885076482\O,-2.0616569333,1.9937484437,-3.2193375481\H,
-2.2287955888,-1.0434855268,0.6733511029\H,-0.5160399306,1.719689323,-
1.1407311584\C,-0.3814873935,-2.0947026541,0.6133426152\C,-0.292319620
7,-2.0716261871,2.0065373153\C,0.654017584,-2.694343994,-0.1114588046\
C,0.816398223,-2.6068430224,2.6621901164\H,-1.0960415992,-1.6043783441
,2.5812858777\C,1.7625221202,-3.230793984,0.5367748701\H,0.6009491967,
-2.725242094,-1.203160138\C,1.8511271122,-3.1822543799,1.9284586275\H,
0.8720048339,-2.5711035709,3.7515433399\H,2.5652451007,-3.685832597,-0.
0459128833\H,2.7220502981,-3.5972079694,2.4377168245\C,-1.3341685333,
1.4249535034,0.7858312436\C,-2.6116383225,1.9329702451,0.5141903798\C,
-0.9127983486,1.3702497886,2.1152650514\C,-3.4469421625,2.3632696117,1.
.5395613296\H,-2.9500014352,1.989635627,-0.5247009959\C,-1.748086623,1.
.8011477955,3.1481886354\H,0.0782708984,0.9815520543,2.3552891262\C,-3.
.0174303071,2.2962858011,2.8658202179\H,-4.4372788319,2.7567987394,1.3
041820695\H,-1.3986570097,1.7501857782,4.1809851052\H,-3.6690318507,2.
6341745125,3.6728922789\Version=ES64L-G09RevE.01\HF=-884.7990065\S2=0.
383261\S2-1=0.\S2A=0.003292\RMSD=8.836e-09\RMSF=3.405e-06\Dipole=-0.0
243698,-0.0488374,-0.389651\Quadrupole=0.6340558,-6.4552418,5.821186,-
4.0664603,2.0843719,-0.3108239\PG=C01 [X(C17H20O3)]\@

TS1a

1\1\GINC-R222\FTS\UM11\6-31+G(d,p)\C17H20O3\ROOT\15-Apr-2016\0\#\ um1
1/6-31+g(d,p) int=ultrafine opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tig
ht,maxcyc=200) nosymm freq=noraman # guess=read geom=allcheck iop(1/8=
1)\TS for O3 H abstraction of pStyrene (pos. b)\O,1\C,1.6517404231,-
1.1684927437,0.3265973852\C,0.681697163,-0.7573457681,1.4563171274\C,2.
.2717683073,-2.5339275406,0.659404492\C,-0.1193825112,0.527975521,1.24
1732599\H,1.2514636864,-0.6621520159,2.3999892639\H,2.954559227,-2.857
6593982,-0.1368654209\H,2.8471872101,-2.4848306191,1.5959568563\H,1.49
19084612,-3.2987885562,0.781768192\H,-0.0215344547,-1.5917638147,1.594
4544112\O,-0.5183375883,0.6946564154,-1.3089302252\O,-0.054356985,1.93
02736281,-1.5563372248\O,-0.8967564738,2.8440070588,-1.2845796487\H,-0.
.3926996123,0.5259094106,0.0357907568\H,1.0606914352,-1.2700914392,-0.
5967984226\C,0.6496355192,1.8399510213,1.4034788929\H,1.1509530107,1.8
399007697,2.3851008478\H,1.4256437553,1.9736248333,0.6382794808\H,-0.0
353480362,2.6963876817,1.3667811941\C,-1.467884302,0.5601601451,1.9118
906934\C,-1.7567886217,-0.2306895847,3.0302485546\C,-2.4553708906,1.43
36123719,1.4346847831\C,-2.995364817,-0.1405738069,3.6630631618\H,-1.0
021491675,-0.9096490642,3.4300074445\C,-3.6951342079,1.5140800898,2.05
87881885\H,-2.2471542549,2.0376171271,0.5477776331\C,-3.9695048533,0.7
278139852,3.1778280908\H,-3.1977090804,-0.7549388037,4.5416968004\H,-4.
454673749,2.1910594999,1.6652237578\H,-4.9415773657,0.7913857836,3.66
86684071\C,2.7268637998,-0.1297829926,0.0650960013\C,2.8143030866,0.50
66987611,-1.1740194079\C,3.6319730447,0.2310711158,1.0690399043\C,3.76
40377872,1.5029672338,-1.3998635631\H,2.1103744807,0.2323512993,-1.963
4341477\C,4.5820055354,1.2236692447,0.8491013545\H,3.5812148923,-0.259
1271658,2.0452913165\C,4.6461870998,1.8691625017,-0.3865422642\H,3.808

4469753,1.9987922676,-2.3707586728\H,5.2742737156,1.499714637,1.646181
6882\H,5.3852973553,2.65285691,-0.5579382814\\Version=ES64L-G09RevE.01
\HF=-884.7787944\S2=0.741863\S2-1=0.\S2A=0.047691\RMSD=6.133e-09\RMSF=
1.268e-06\Dipole=0.3295881,-0.4755511,0.8808397\Quadrupole=1.942808,-3
.9753307,2.0325228,2.181511,-1.5918474,-1.4606205\PG=C01 [X(C17H2003)]
\@

TS1b

1\1\GINC-R63\FTS\UM11\6-31+G(d,p)\C17H2003\ROOT\09-Apr-2016\0\\# um11/
6-31+g(d,p) int=ultrafine opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,
maxcyc=200) nosymm freq=noraman # guess=read geom=allcheck iop(1/8=1
)\TS for O3 H abstraction of pStyrene (pos. a)\0,1\C,1.7197374235,-0
.9106802578,0.4100524127\C,1.1749741898,0.5113962384,0.2938879122\C,0.
8605814028,-1.9528096455,-0.3147960019\C,0.7159117066,1.0121724878,-1.
0714843791\H,1.8158142455,1.2429184712,0.8135214178\H,1.2534523468,-2.
9617154683,-0.1328767596\H,-0.1866170112,-1.92718643,0.0148523756\H,0.
8627625336,-1.7783092649,-1.3989730111\H,0.1561301236,0.5867011373,1.0
441927315\O,-0.9125813448,0.7280014162,1.7697449673\O,-1.6060456004,-0
.4164029615,1.5836083336\O,-2.1155973534,-0.4985649491,0.4185213449\H,
-0.096016718,0.3573217778,-1.4245371846\H,2.7071325189,-0.8846368127,-
0.0894414855\C,1.8824609051,0.9324633642,-2.0770129985\H,2.7739305131,
1.4523614292,-1.6969547308\H,2.165213154,-0.1102701015,-2.2751244928\H
,1.5950310539,1.4007168123,-3.0273211184\C,0.1519055578,2.420364109,-0
.9525360131\C,-1.2295661325,2.6228476517,-0.9404596523\C,0.9943375328,
3.5277174013,-0.8190000112\C,-1.7593891811,3.9047136625,-0.8099836041\
H,-1.8936459941,1.7589495388,-1.0151407856\C,0.468448672,4.8108899901,
-0.6870331668\H,2.0785744771,3.3913983392,-0.8197519208\C,-0.911860270
3,5.003235883,-0.6851238408\H,-2.8414301698,4.0441437987,-0.8016570976
\H,1.1405412488,5.6645350436,-0.5861436866\H,-1.3253002432,6.007566941
8,-0.5832254991\C,1.9853253874,-1.2375269262,1.8736559518\C,3.14347760
3,-0.7477890519,2.4847623058\C,1.0854141457,-1.9773519637,2.6428541282
\C,3.3997818353,-0.9872231713,3.8316339218\H,3.8586284506,-0.172406381
3,1.88964489\C,1.3379383749,-2.2194662925,3.9925547066\H,0.1746493359,
-2.3723331975,2.1895829076\C,2.4938095079,-1.7257004232,4.5914502548\H
,4.3114915709,-0.5995598542,4.2886850454\H,0.6225379045,-2.7979439373,
4.5789513108\H,-2.690226297,-1.9171714038,5.6471465223\\Version=ES64L-G
09RevE.01\HF=-884.7716352\S2=0.786091\S2-1=0.\S2A=0.046734\RMSD=3.774e
-09\RMSF=8.060e-07\Dipole=0.9972607,-0.0326503,-0.3025596\Quadrupole=1
.8598462,-0.0233701,-1.8364761,1.8911548,1.2572148,-1.2662903\PG=C01 [X
(C17H2003)]\@

int-2 (rad)

1\1\GINC-R162\FOpt\UM11\6-31+G(d,p)\C17H19(2)\ROOT\10-Jun-2016\0\\# um
11/6-31+g(d,p) opt=maxcyc=200 scf=(tight,maxcyc=200) freq=noraman int=
ultrafine\pStyrene-C* (tertiary)\0,2\C,-1.2257324586,0.2714112152,0.
7241581672\C,-0.3375399287,1.3080298116,-0.0196071363\C,-0.6081857667,
-1.131961516,0.6690597038\C,1.000037687,1.499762324,0.6338045411\H,-0.
873289317,2.2717907072,-0.0213199567\H,-1.2292418083,-1.8537426674,1.2
159275202\H,-0.5230274653,-1.4834125099,-0.3703464432\H,0.4010382667,-
1.1332629601,1.1037585715\C,1.0127509349,2.3084620747,1.9008314474\H,0
.0013887657,2.6517279785,2.1550049987\H,1.3963324457,1.729835383,2.757
2778763\H,1.6519281665,3.2020144228,1.8075721894\H,-0.2452046715,1.005
7036602,-1.0722556844\H,-1.2817878164,0.5818217611,1.7808861885\C,2.20
94427169,0.9240837165,0.137550419\C,3.4489355071,1.1627489926,0.792419
7934\C,2.2472025982,0.0874844777,-1.0111378321\C,4.6329726885,0.611178
1611,0.3272013027\H,3.4736515667,1.7964780156,1.6789100211\C,3.4354208
662,-0.4604690238,-1.4678183298\H,1.3250351516,-0.1418964688,-1.544242
6865\C,4.6405261846,-0.204777355,-0.8068148647\H,5.5653541434,0.819236
5407,0.8547604068\H,3.4250865467,-1.0999262461,-2.352055112\H,5.572679
6317,-0.6378853983,-1.1703364554\C,-2.6382160117,0.2918294608,0.167778
1986\C,-2.8953697448,-0.104678339,-1.1493530993\C,-3.7104922428,0.7237
931424,0.9509310857\C,-4.1868975252,-0.0706023274,-1.6675479883\H,-2.0
716425738,-0.4467928118,-1.7813664609\C,-5.0070744019,0.7583579016,0.4
384751922\H,-3.5254385523,1.0364954027,1.9816800106\C,-5.249372068,0.3
611738292,-0.8737440607\H,-4.3663399905,-0.3836726567,-2.6973932801\H,
-5.8305485479,1.0972001216,1.0692088573\H,-6.2620719768,0.3869191795,-
1.2783061011\\Version=ES64L-G09RevE.01\State=2-A\HF=-658.8152835\S2=0.
79767\S2-1=0.\S2A=0.751436\RMSD=9.146e-09\RMSF=3.364e-06\Dipole=-0.130

3885,0.0931121,0.1877993\Quadrupole=1.9278633,-4.2781974,2.3503341,-1.3691559,1.0860561,5.0033511\PG=C01 [X(C17H19)]\@

hydrotrioxide

1\1\GINC-R55\FOpt\RM11\6-31+G(d,p)\C17H20O3\ROOT\03-Apr-2016\0\# m11/
6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noraman
\Intm 2 'zwitterionic' - OOH pos. b\0,1\C,0.1393016031,-1.9041912986
,0.2278758166\C,0.9869603828,-1.44328601,-0.9744006392\C,-0.1003536556
, -3.4207747145,0.1345514591\C,1.8626542935,-0.1999466373,-0.7453714362
\H,0.3449208922,-1.2293821138,-1.8425232467\H,-0.7188162685,-3.7748469
748,0.9704259132\H,-0.6256126673,-3.6698217563,-0.8003719358\H,0.85901
01489,-3.9558116805,0.1461977484\C,1.0878779057,0.9460060912,-0.101852
9878\H,0.7003603883,0.6256279646,0.871001377\H,1.742347482,1.811055575
7,0.0613160946\H,0.2360401318,1.2363730673,-0.7316055123\H,1.643088855
9,-2.2708667741,-1.2782126571\O,3.127945959,-2.6868624029,0.6351495501
\O,3.6593909928,-1.5642968918,-0.0363586021\O,2.8608005013,-0.46362633
19,0.2970798416\H,3.5582545988,-2.6312445376,1.5038080367\H,0.72027244
8,-1.7073536715,1.1430988627\C,2.5608235639,0.2015955646,-2.0513335567
\C,3.2700459824,-0.7479118674,-2.79999312\C,2.4892821487,1.5065442046,
-2.5464898777\C,3.899286591,-0.3967353652,-3.9907073542\H,3.3466008327
, -1.7747649538,-2.4449346956\C,3.1129932919,1.8594041968,-3.742793964\
H,1.9354666198,2.2714835745,-2.0036947033\C,3.823700336,0.9097980517,-
4.4690851835\H,4.4513979813,-1.1536002141,-4.5499520096\H,3.0385933115
,2.8856602134,-4.105665009\H,4.3138595264,1.1838713295,-5.4043652825\C
, -1.1981383567,-1.1861939064,0.3505671771\C,-2.0811206774,-1.113619904
9,-0.7314627514\C,-1.6018245818,-0.6329960046,1.5684411854\C,-3.321163
8418,-0.4915868476,-0.60581861\H,-1.800072675,-1.5558056367,-1.6907206
035\C,-2.8411299723,-0.0095215283,1.7022615444\H,-0.9250759422,-0.6862
396685,2.4259580749\C,-3.7052041902,0.067067092,0.6121322376\H,-3.9925
967105,-0.4443940718,-1.4647924348\H,-3.1310525194,0.4204543843,2.6624
440809\H,-4.6747711911,0.5568809949,0.7114344824\Version=ES64L-G09Rev
E.01\State=1-A\HF=-884.8883648\RMSD=5.624e-09\RMSF=5.968e-06\Dipole=-0
.225523,0.0696366,0.1484761\Quadrupole=-3.586957,-1.3126584,4.8996153,
-4.025491,0.1375478,-2.0313393\PG=C01 [X(C17H20O3)]\@

TS2a

1\1\GINC-R265\FTS\UM11\6-31+G(d,p)\C17H20O3\ROOT\13-May-2016\0\# um11/
6-31+g(d,p) int=ultrafine opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tig
ht,maxcyc=200) nosymm freq=noraman # guess=read geom=allcheck\TS for
for peroxy radical addition to *OpStyrene pos. b\0,1\C,1.4754425837,
0.4395817103,0.9341171624\C,0.2056767468,-0.097977405,0.2447376061\C,1
.5595848049,1.9737787716,0.9502340142\C,-1.1590319832,0.2648943053,0.8
753859282\H,0.2728220205,-1.1954716249,0.2123995147\H,2.5414359209,2.2
958762323,1.3234797803\H,1.4245237654,2.3809354562,-0.0620997525\H,0.7
74251458,2.41293228,1.576574018\C,-1.1693126014,-0.014606737,2.4033829
616\H,-0.4598291909,0.645008094,2.9180230462\H,-2.1758786538,0.1467005
019,2.8062995039\H,-0.8788665661,-1.0608092642,2.5712244993\H,0.183736
8919,0.2429773128,-0.8010700053\O,-0.7394041113,3.5045797878,-0.918484
3466\O,-1.1864789875,2.2715822575,-1.0606054623\O,-1.4145108204,1.6350
542154,0.8387250741\H,-1.5318315043,4.0587670907,-0.7992739458\H,1.491
6067497,0.0736452612,1.9736137371\C,-2.2844786593,-0.5342043628,0.2059
256115\C,-2.2690173746,-1.9328078165,0.2210873206\C,-3.3525832391,0.11
892565,-0.4083517815\C,-3.2961312056,-2.6631023003,-0.3693983979\H,-1.
446872723,-2.4661823878,0.70450599\C,-4.381132114,-0.6112031816,-1.003
6904417\H,-3.3701166176,1.2081525903,-0.415794813\C,-4.3570644063,-2.0
028489825,-0.9879297884\H,-3.2674398822,-3.7535779647,-0.3464367415\H,
-5.2076819416,-0.0849564214,-1.4840585249\H,-5.1618119634,-2.573188238
8,-1.4538787783\C,2.6893866048,-0.1638292002,0.2426687628\C,3.00688881
07,0.184381477,-1.0750140539\C,3.5037244538,-1.0884505232,0.8990993422
\C,4.1084621335,-0.3754678575,-1.7158155684\H,2.3816260885,0.906085846
8,-1.6068469884\C,4.609643466,-1.6520165472,0.2627583708\H,3.268514272
3,-1.3689840733,1.9290430037\C,4.9152632497,-1.2970448207,-1.048292256
\H,4.3397157687,-0.0910196506,-2.743692074\H,5.2343500952,-2.370835134
4,0.7956380047\H,5.7793126608,-1.7352643466,-1.5497135317\Version=ES6
4L-G09RevE.01\HF=-884.8479118\S2=0.732698\S2-1=0.\S2A=0.018379\RMSD=3.
575e-09\RMSF=7.622e-07\Dipole=-0.4402474,0.222048,0.1637139\Quadrupole
=-2.3678109,4.8826967,-2.5148858,-5.8949218,1.9379695,-3.4661996\PG=C0
1 [X(C17H20O3)]\@

alkoxyl

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1\1\GINC-R559\FOpt\UM11\6-31+G(d,p)\C17H19O1(2)\ROOT\21-May-2016\0\#\#
m11/6-31+g(d,p) opt=(maxcyc=200) freq=noraman nosymm scf=(tight,maxcyc
=200) int=ultrafine\pStyrene-O* (tertiary)\0,2\C,-1.4067422967,0.052
1194081,1.1598115979\C,-0.1117945231,0.208998835,0.3447612178\C,-1.571
4594873,-1.3482045808,1.767187266\C,1.2527156213,0.0242200475,1.122885
2745\H,-0.0632209144,1.2227321639,-0.0814748205\H,-2.5730600524,-1.462
0293826,2.2029224578\H,-1.4400879793,-2.1262587519,1.0007144375\H,-0.8
200234372,-1.5344046798,2.5442295247\C,1.2458743055,0.8337816015,2.428
5697274\H,0.5648711311,0.3552091925,3.1431057609\H,2.2523496389,0.8562
178183,2.8659979036\H,0.9096661832,1.8667666599,2.2635548287\H,-0.1048
251743,-0.497797026,-0.4997363201\O,1.3135949554,-1.3232263656,1.37887
6936\H,-1.3944534913,0.7912844112,1.976456008\C,2.3653841676,0.4409594
334,0.1484137094\C,2.8318580445,1.7559627897,0.0992520695\C,2.88842055
15,-0.4993222414,-0.7403994399\C,3.8086266613,2.1249085197,-0.82434907
25\H,2.4353134,2.5063899412,0.7853712615\C,3.8647354607,-0.1311530237,
-1.6631828791\H,2.5283380642,-1.5277080725,-0.6907263582\C,4.328299022
,1.1823869267,-1.7084544169\H,4.1655699185,3.1556329627,-0.8502520147\
H,4.2683026971,-0.8772263363,-2.3495554281\H,5.0942834662,1.4706092739
,-2.4296378844\C,-2.5758474977,0.4149218693,0.2543892672\C,-2.95931422
86,-0.4301983384,-0.7923073314\C,-3.2736140614,1.6110568216,0.43273607
92\C,-4.0134512172,-0.0895307011,-1.6352908645\H,-2.4263966355,-1.3711
120949,-0.9501112789\C,-4.3312532114,1.9570252586,-0.4077123142\H,-2.9
851871152,2.2808166689,1.2469145174\C,-4.7042530559,1.1069458067,-1.44
54432502\H,-4.2983253979,-0.7624249205,-2.4456648886\H,-4.8658190519,2
.8949201907,-0.2487374742\H,-5.5313204604,1.3739279142,-2.1046288086\
Version=ES64L-G09RevE.01\HF=-733.9867079\S2=0.753521\S2-1=0.\S2A=0.750
008\RMSD=7.394e-09\RMSF=5.483e-06\Dipole=-0.1852262,0.690251,-0.153219
\Quadrupole=-0.8544772,1.0198802,-0.165403,1.2644078,-1.2072555,4.8734
348\PG=C01 [X(C17H19O1)]\@
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TS3a

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1\1\GINC-R2020\FTS\UM11\6-31+G(d,p)\C17H19O1(2)\ROOT\21-May-2016\0\#\#
m11/6-31+g(d,p) opt=(ts,calcf, noeigen,maxcyc=200) freq=noraman nosymm
scf=(tight,maxcyc=200) int=ultrafine\TS for C-Calpha fragmentation :
pPropylene-O* (tertiary)\0,2\C,1.7040934217,0.6294824328,0.736605708
2\C,0.4831593293,0.0037783461,0.1123815067\C,1.6357727562,2.1598484677
,0.7951309494\C,-1.2336669061,0.4237510502,1.2080755219\H,0.426416598,
-1.0883388019,0.1436369088\H,2.6064032433,2.5738533836,1.0985350302\H,
1.3699504307,2.5787961941,-0.1858524099\H,0.8582051882,2.4856679744,1.
495335766\C,-0.7600611953,-0.0127614142,2.5943185867\H,-0.1192220618,0
.7746871069,3.0074406864\H,-1.6430268308,-0.1174055671,3.2417228609\H,
-0.2174112575,-0.9670171916,2.5933061276\H,0.1469438906,0.4393057398,
-0.8333926124\O,-1.3461657647,1.6505268537,0.9726596146\H,1.8272019971,
0.2310053558,1.7560525563\C,-2.1203237684,-0.5408351514,0.4349633959\C
,-2.2533145361,-1.8851439486,0.7895940978\C,-2.8283005588,-0.047278949
6,-0.6624614135\C,-3.0847851918,-2.7267514445,0.0527467341\H,-1.710999
6807,-2.2855050611,1.648151691\C,-3.6562654541,-0.8879013102,-1.399931
1242\H,-2.719993706,1.0100156809,-0.9099411258\C,-3.7857696055,-2.2306
664122,-1.0445183151\H,-3.1860142385,-3.7747031498,0.3388607984\H,-4.2
082232776,-0.4936413282,-2.2545576534\H,-4.4360646006,-2.8900159124,-1
.6211975019\C,2.8933550226,0.1201430375,-0.0794685579\C,3.1711361665,0
.6420288351,-1.3469598121\C,3.7019729899,-0.9060874121,0.414502535\C,4
.2390561884,0.1561369686,-2.0966097899\H,2.5465412332,1.4413905549,-1.
7517300134\C,4.7726817751,-1.3943168962,-0.3322574107\H,3.4933035958,-
1.3222182791,1.4033697145\C,5.0444601508,-0.8636818809,-1.5911220959\H
,4.4442256347,0.5769229265,-3.0821646079\H,5.3983297586,-2.1909429918,
0.0732818083\H,5.8824322636,-1.2426358057,-2.1775891548\Version=ES64L
-G09RevE.01\HF=-733.9719649\S2=0.768781\S2-1=0.\S2A=0.750088\RMSD=6.03
9e-09\RMSF=2.378e-06\Dipole=0.5759933,-1.079493,-0.1025004\Quadrupole=
-0.3860808,-2.6030954,2.9891762,2.287724,1.9056476,-4.566264\PG=C01 [X
(C17H19O1)]\@
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CH₃COR¹

```
1\1\GINC-R271\FOpt\RM11\6-31+G(d,p)\C8H8O1\ROOT\14-Jun-2016\0\#\# m11/6
-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=noram
an\beta-scission acetone fragment\0,1\C,-1.7869763417,1.454649018,0.
```

1905150521\C, -1.3034299458, 1.883474345, 1.5597171576\H, -0.7072167748, 2.793973307, 1.450776279\H, -2.1556182133, 2.0766291753, 2.2261061452\H, -0.6921718525, 1.093265628, 2.0174569286\O, -1.4995203484, 2.0951641681, -0.8038396052\C, -2.6336580469, 0.2165821653, 0.0786388838\C, -2.9858551154, -0.54640492, 1.1947183237\C, -3.0732913153, -0.1680498184, -1.1909618361\C, -3.7724111161, -1.6860846081, 1.0418341927\H, -2.6485453458, -0.2560256637, 2.1909022658\C, -3.8580536439, -1.3051512144, -1.3433914976\H, -2.7830517545, 0.4464789467, -2.0442152205\C, -4.2081214304, -2.0650472, -0.2262599861\H, -4.0456914473, -2.2796531335, 1.9150605826\H, -4.1998107784, -1.6029205607, -2.3354813509\H, -4.8240795096, -2.9577336346, -0.3454082949\Version=ES64L-G09RevE.01\State=1-A\HF=-384.6812319\RMSD=3.640e-09\RMSF=6.679e-06\Dipole=-0.4242798, -0.8252901, 0.9052244\Quadrupole=-1.3331305, -1.7353088, 3.0684393, 1.0750211, 3.3377341, 3.7810286\PG=C01 [X(C8H8O1)]\@\

ROOH

1\1\GINC-R342\FOpt\RM11\6-31+G(d,p)\C9H12O2\ROOT\26-Jun-2016\0\#\ m11/6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=noraman\beta-scission C fragment peroxide\0,1\C, 1.6894062911, -0.4041431866, 0.1354180185\C, 2.3838195833, -0.2143081388, -1.2199025037\H, 1.9330847538, -0.8657949775, -1.979881888\H, 2.2913163864, 0.8258207163, -1.565301925\H, 3.4530020582, -0.4461529298, -1.1403518327\H, 1.8674180639, -1.4334347866, 0.4833448559\C, 0.1872932201, -0.1891079696, 0.05713095\C, -0.340958037, 1.0044593147, -0.4464771071\C, -0.6974335698, -1.1730036861, 0.5034976133\C, -1.7173808451, 1.2069615255, -0.5039651267\H, 0.3327856944, 1.787772265, -0.802297856\C, -2.0763653948, -0.976347401, 0.4458891421\H, -0.297667783, -2.1091721309, 0.9005431934\C, -2.5906008711, 0.2155860712, -0.0582268646\H, -2.1109569021, 2.144399442, -0.900080451\H, -2.7507846975, -1.7589667185, 0.7968526354\H, -3.6690123943, 0.372776351, -0.1047798939\C, 2.2699389095, 0.5397977677, 1.1914896355\H, 2.1601806576, 1.5942539667, 0.8837947073\H, 1.780079344, 0.3993073587, 2.1682444019\O, 3.6517156874, 0.2321743412, 1.3087362625\O, 4.1513424097, 1.1407150143, 2.2957244978\H, 5.0815086153, 0.8749288195, 2.323239259\Version=ES64L-G09RevE.01\State=1-A\HF=-500.2733191\RMSD=5.889e-09\RMSF=4.513e-06\Dipole=0.0014208, -0.1453982, -0.1435145\Quadrupole=5.2328739, -0.6524205, -4.5804534, -0.3666608, 0.8645867, -2.8072749\PG=C01 [X(C9H12O2)]\@\

Poly(methyl acrylate)

pMA

1\1\GINC-R63\FOpt\RM11\6-31+G(d,p)\C9H16O4\ROOT\03-Apr-2016\0\#\ m11/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noraman\MA\0,1\C, -0.1925435647, -1.3139251763, 0.3320802243\C, -0.7846038851, 0.007742688, 0.83560074\H, -1.8467528443, -0.1534315546, 1.0763684234\H, -0.2734330845, 0.2962440587, 1.7679462092\C, -0.7077306488, 1.1790108842, -0.1684542605\C, 0.7497171316, 1.4504767192, -0.489806238\C, 1.3239658545, -1.2495709775, 0.3119362139\O, 1.3323706027, 2.2673579148, 0.3932039767\O, 1.8531446706, -1.9953371144, -0.6620412785\C, 2.7538909319, 2.4061637232, 0.2572044326\H, 3.0003782414, 2.7778353866, -0.7450157441\H, 3.2239814547, 1.4279713935, 0.421786767\H, 3.0592849188, 3.1204045151, 1.0268364571\C, 3.2727258358, -1.872748176, -0.8181924928\H, 3.7840282556, -2.1689664752, 0.1060047664\H, 3.5141816954, -0.8284165237, -1.0581614506\H, 3.5421945151, -2.5336827096, -1.64641304\O, 1.3513103789, 0.9383561479, -1.4146194495\O, 1.9973014267, -0.6209418176, 1.1051905329\C, -0.5996335471, -2.4862196156, 1.2415898498\H, -0.1567188937, -3.429213909, 0.8952247218\H, -1.6918623861, -2.5990771285, 1.2481491374\H, -0.2644667095, -2.2999276242, 2.2717658299\C, -1.4274964071, 2.4124733802, 0.3813737151\H, -2.490896827, 2.1860832373, 0.5382418579\H, -1.3552064038, 3.2627424297, -0.3094332203\H, -0.9891217327, 2.715923131, 1.3406214778\H, -1.1599159599, 0.8581241405, -1.1180622645\H, -0.5213250196, -1.5155189476, -0.6979558949\Version=ES64L-G09RevE.01\State=1-A\HF=-653.2232167\RMSD=4.356e-09\RMSF=3.972e-06\Dipole=-0.2968509, -0.0835898, 0.1490706\Quadrupole=5.3897425, 1.5009843, -6.8907268, 0.4067999, -1.6444432, 0.3469046\PG=C01 [X(C9H16O4)]\@\

int-1

1\1\GINC-R626\FOpt\UM11\6-31+G(d,p)\C9H16O7\ROOT\26-Aug-2015\0\#\um11/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noraman #guess=read geom=allcheck\O3 + pMA caged complex\0,1\C, -0.2342285546, 1.1534267532, -0.4001810757\C, -0.6611969499, -0.209107651, -0.958304119

7\H,-1.7390285444,-0.1775642673,-1.1872617188\H,-0.1346508494,-0.38925
25894,-1.9089929237\C,-0.4063582243,-1.3992535655,-0.00680916\C,1.0824
923138,-1.4731285338,0.2775093497\C,1.273885211,1.3110392149,-0.469492
249\O,1.7504411209,-2.1868756703,-0.6331467392\O,1.7422496421,2.122652
0356,0.4833795927\C,3.1805551813,-2.1291829404,-0.529283659\H,3.499658
403,-2.4917093644,0.4556453751\H,3.5058209794,-1.0905072264,-0.6707649
574\H,3.5639730292,-2.7710519613,-1.327183391\C,3.1705293812,2.2111122
539,0.5588797037\H,3.5794750397,2.5842722262,-0.3881286749\H,3.5783515
405,1.2133909511,0.7708874648\H,3.3862250336,2.9005792634,1.3795909668
\O,1.6285450483,-0.8960097683,1.1981862547\O,1.9882266024,0.7897769875
, -1.3036783214\C,-0.8772403415,2.3051958384,-1.1911587485\H,-0.5501913
928,3.2802633853,-0.8071843389\H,-1.970944696,2.2469575469,-1.10972629
14\H,-0.603437821,2.236912799,-2.253666643\C,-0.9623368616,-2.69867409
32,-0.5931219496\H,-2.0487581328,-2.6153989441,-0.7364200123\H,-0.7663
127292,-3.5550157551,0.065338002\H,-0.4999657466,-2.9054410575,-1.5665
873512\O,-3.4924546494,-0.554546288,0.860532384\O,-3.0375423713,0.6177
05383,0.9518919429\O,-4.0148166823,-0.8617796867,-0.2448732259\H,-0.86
84215496,-1.1792934722,0.9680402291\H,-0.5136268399,1.2393489964,0.660
8103551\\Version=ES64L-G09RevD.01\State=1-A\HF=-878.5629915\S2=0.38658
1\S2-1=0.\S2A=0.003371\RMSD=6.839e-09\RMSF=7.607e-06\Dipole=-0.2592149
, -0.0810691,0.028257\Quadrupole=5.2705966,1.3946145,-6.665211,0.621494
4,-0.8085436,0.3185591\PG=C01 [X(C9H16O7)]\@

TS1a

1\1\GINC-R3456\FTS\UM11\6-31+G(d,p)\C9H16O7\ROOT\26-Aug-2015\0\#um11/
6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcfc,noeigen,maxcyc
=200) freq=noraman #guess=read geom=allcheck\TS for O3 H abstraction
of pMA\0,1\C,0.341564154,-1.5956361785,-0.3155568352\C,-0.6918329839,
-0.6767479587,0.3399498574\C,0.0798049444,-3.0694381029,0.0367497279\C
1.7401308502,-1.2221053854,0.1428607885\C,-0.7443416604,0.7561697387,
-0.1871959663\H,-0.4856711331,-0.6244605426,1.423197468\H,0.8451523447
, -3.7174345267,-0.4079912053\H,0.0878464914,-3.2150356547,1.1266076153
\H,-0.9015785681,-3.3805271857,-0.3445282738\O,2.680578567,-1.73367941
27,-0.6552780231\O,1.9972302976,-0.552805271,1.1251470791\C,-1.7778814
329,1.6397068712,0.4744768627\C,0.6114088347,1.3793293405,-0.408883454
3\C,4.0218374686,-1.3236101965,-0.3612602664\H,-1.8499125844,2.6120015
552,-0.0268680044\H,-2.7623620434,1.1542293436,0.4547827542\H,-1.49194
72002,1.8111139417,1.5234037214\O,0.8956931564,2.3349444186,0.47430281
65\O,1.3696190422,1.0296708502,-1.292805922\H,4.0952389204,-0.23276028
53,-0.4655733306\H,4.2924690076,-1.6133186103,0.6613854388\H,4.6577290
504,-1.8263468486,-1.0947964916\C,2.2343301724,2.8504981536,0.39680394
33\H,2.3040005516,3.6167144065,1.1732382074\H,2.9410852788,2.032078017
3,0.5867175586\H,2.4136387394,3.2754956016,-0.5979983062\H,-1.69523810
17,-1.113281051,0.2209353926\O,-1.493193447,0.5174119134,-2.6134660045
\O,-0.7553899131,1.4859765235,-3.202720947\O,-1.0520026851,2.641399054
2,-2.7723565819\H,-1.1322592704,0.597060578,-1.3835374541\H,0.32625315
2,-1.4716130973,-1.408742165\\Version=ES64L-G09RevD.01\State=1-A\HF=-8
78.5338656\S2=0.770844\S2-1=0.\S2A=0.04484\RMSD=3.877e-09\RMSF=3.803e-
06\Dipole=0.2943406,-0.4463487,0.8968784\Quadrupole=5.7842129,2.373452
5,-8.1576654,2.8180579,-3.2283247,2.9146787\PG=C01 [X(C9H16O7)]\@

TS1b

1\1\GINC-R1915\FTS\UM11\6-31+G(d,p)\C9H16O7\ROOT\26-Aug-2015\0\#um11/
6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcfc,noeigen,maxcyc
=200) freq=noraman #guess=read geom=allcheck nosymm iop(1/8=1)\TS for
O3 H abstraction of pMA\0,1\C,-0.6210362948,-1.2149954478,0.37272738
05\C,-0.7889144364,0.277226967,0.6158192186\C,-1.1795173049,-2.0430336
241,1.5380191883\C,0.8763244418,-1.4815061707,0.237278964\C,-0.3459617
052,1.230722768,-0.4873087544\H,-0.4413568137,0.5894124635,1.612640187
5\H,-1.0676115115,-3.1174352419,1.3452001105\H,-0.6384934931,-1.795380
1266,2.4613065911\H,-2.2458493938,-1.8256771043,1.6823244905\O,1.19247
73672,-2.0843663934,-0.9058666719\O,1.6909877927,-1.1578173263,1.07854
18575\C,-0.9890208507,2.616032083,-0.3307583042\C,1.1769188436,1.32950
5808,-0.4329716877\C,2.6017218484,-2.2551029805,-1.1420064154\H,-0.601
6772782,3.3137291587,-1.0841267949\H,-2.0754717463,2.531625355,-0.4586
397493\H,-0.7742171204,3.0258668826,0.6650713812\O,1.6000234999,1.9051
726188,0.6962163592\O,1.9260438849,0.9085315751,-1.2886478856\H,3.0453
845116,-2.8479017876,-0.3330327498\H,2.679600242,-2.7742900644,-2.1006

252202\H,3.0743623695,-1.2660018044,-1.1900961127\C,3.0207405938,1.86805566,0.9065504522\H,3.1935410568,2.3676218398,1.8638128461\H,3.3461708587,0.8210313647,0.9442908565\H,3.533695069,2.3925608795,0.0909159454\H,-2.0490496353,0.433918971,0.7347903949\O,-3.3285210928,0.4065611828,0.7106104914\O,-3.5768017266,-0.4380556148,-0.3273532273\O,-3.2260241481,0.0606759801,-1.4433677676\H,-0.589003209,0.7998953238,-1.4679636886\H,-1.0973526191,-1.4974021004,-0.5767626861\Version=ES64L-G09RevD.01\HF=-878.533619\S2=0.811477\S2-1=0.\S2A=0.050566\RMSD=5.728e-09\RMSF=6.801e-07\Dipole=0.6355554,-0.0627553,0.4111557\Quadrupole=-1.6679405,5.3467816,-3.678841,0.68195,-0.9823415,1.8545087\PG=C01 [X(C9H1607)]\@

int-2 (rad)

1\1\GINC-R368\FOpt\UM11\6-31+G(d,p)\C9H1504(2)\ROOT\10-Jun-2016\0\#\ um11/6-31+g(d,p) opt=maxcyc=200 scf=(tight,maxcyc=200) freq=noraman int=ultrafine\pMA-C* (tertiary)\0,2\C,-0.3898191973,0.4219449391,-0.2965413621\C,-0.5039558699,-0.185726466,1.1023451435\C,0.7374766292,-0.257089709,-1.090953882\C,-0.1006473977,1.9053083503,-0.1889152106\C,-1.5172997929,0.3625835735,2.0593517878\H,0.4794661933,-0.0950998515,1.5980232388\H,0.8233701733,0.1798692029,-2.0936061643\H,1.7023990285,-0.1420607982,-0.5758892393\H,0.5333326399,-1.3312096685,-1.1977918333\O,-0.3171443907,2.542642769,-1.3469872136\O,0.3161502137,2.4646396704,0.8048869254\C,-1.4499095833,-0.0982923308,3.4783039749\C,-2.5093513993,1.3553872806,1.6837659931\C,-0.1328669368,3.9616949207,-1.3039752785\H,-2.4472008239,-0.3230907456,3.8785681148\H,-0.8098548528,-0.985090314,3.5706858432\H,-1.0279840384,0.696485771,4.1156667363\O,-3.2709632882,1.745895141,2.7351583928\O,-2.6843503956,1.8183974923,0.562669357\H,-0.8224248044,4.3979249771,-0.5700365768\H,0.8986141449,4.2022757828,-1.0176603185\H,-0.3550610955,4.325092972,-2.3111864838\C,-4.255492197,2.7370150288,2.430885444\H,-4.9518225757,2.3594978171,1.6712777929\H,-4.7764213323,2.9410610117,3.3709024169\H,-3.7712470315,3.6443827385,2.0481458985\H,-0.6811382797,-1.2726123405,1.0011118434\H,-1.3340297399,0.3267577902,-0.8458483406\Version=ES64L-G09RevE.01\State=2-A\HF=-652.5703737\S2=0.75612\S2-1=0.\S2A=0.750023\RMSD=4.769e-09\RMSF=6.582e-06\Dipole=-0.1822873,-0.3843564,0.1367527\Quadrupole=-1.6967741,3.2978431,-1.6010691,-3.0626831,-4.3810579,-2.2311508\PG=C01 [X(C9H1504)]\@

hydrotrioxide

1\1\GINC-R2563\FOpt\RM11\6-31+G(d,p)\C9H1607\ROOT\01-Apr-2016\0\#\ m11/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noraman\Intm 2 'zwitterionic' - OOH pos. b\0,1\C,1.0519618316,-0.9193512219,-0.3195812412\C,0.3006198999,-0.9921852304,1.0125536205\C,2.1775405882,-1.9635144679,-0.3847095141\C,1.6318685341,0.4646578867,-0.5399748901\C,-1.1340619635,-0.4353428621,0.9603251119\H,0.8534633841,-0.4330560217,1.782068802\H,2.7338569194,-1.8848932642,-1.3273993496\H,2.8810287956,-1.831196523,0.4500519652\H,1.7401404035,-2.9682207436,-0.3143818021\O,1.9532625805,0.6717057221,-1.8222823843\O,1.8049786334,1.3046309779,0.3224487534\C,-1.8276049018,-0.5342616138,2.3136059393\C,-1.0749439402,0.9998360183,0.4244795955\C,2.4004512219,1.9960130631,-2.1349851352\H,-2.8451817098,-0.128106877,2.2547029673\H,-1.8787267175,-1.587670149,2.6153152131\H,-1.2645039735,0.0303410492,3.0648624201\O,-0.9663363099,1.887955024,1.4116069819\O,-1.0535068141,1.2865395508,-0.7515510225\H,1.6000932822,2.7121886321,-1.9048164675\H,3.2935696461,2.2446550012,-1.5486488005\H,2.6210787846,1.9943243638,-3.2058971198\C,-0.6834816176,3.2329321301,0.9920508908\H,-0.6484123273,3.828231281,1.9082415335\H,0.2854037906,3.2460505365,0.477094504\H,-1.4742781634,3.5876321896,0.3201531029\H,0.2277201351,-2.039992363,1.33828291\O,-1.0365293156,-3.1634679736,-0.4619605835\O,-2.0079684194,-2.4743180836,0.2911004552\O,-1.916780656,-1.1171638802,-0.0523431929\H,-1.4947858478,-3.3139226785,-1.305279422\H,0.3528578465,-1.0955216329,-1.1486260014\Version=ES64L-G09RevE.01\State=1-A\HF=-878.6503018\RMSD=7.599e-09\RMSF=4.236e-06\Dipole=0.2841125,0.0839288,-0.0944887\Quadrupole=-3.7558327,4.2545723,-0.4987396,0.5997533,-3.8251871,2.1829502\PG=C01 [X(C9H1607)]\@

TS2a

1\1\GINC-R177\FTS\UM11\6-31+G(d,p)\C9H1607\ROOT\15-Apr-2016\0\#\ um11/6-31+g(d,p) int=ultrafine opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200) nosymm freq=noraman # guess=read geom=allcheck\TS for f

or peroxy radical addition to *OpMA pos. b\0,1\C,-0.3992810332,0.3567357895,-0.1793833528\C,-0.4083971886,-0.4100604125,1.1535720466\C,0.7438256841,-0.1660199058,-1.054282958\C,-0.3685107942,1.8542742933,0.034281122\C,-1.5513104908,-0.1635505366,2.2233660499\H,0.5392866874,-0.2419400303,1.6845550169\H,0.7594740014,0.3421372346,-2.0245154382\H,1.7190877194,-0.0095186223,-0.5714773102\H,0.6014861191,-1.240851251,-1.2246397009\O,0.3412667707,2.522858708,-0.8794480758\O,-0.9674117216,2.4212126743,0.9309143371\C,-1.0174303487,0.5347332952,3.4756846841\C,-2.7748038192,0.5442249898,1.6165264015\C,0.3346662262,3.9516758057,-0.7442756149\H,-1.7975984067,0.5960813237,4.2432577133\H,-0.1754193602,-0.0497308094,3.8659893594\H,-0.6928332828,1.549648723,3.218047918\O,-3.2598217566,1.5223623046,2.3546706796\O,-3.3062350105,0.1722355129,0.5785188306\H,-0.6914111039,4.3300292851,-0.8279990749\H,0.7439365545,4.2367901589,0.2323944672\H,0.9592332096,4.3307079533,-1.5574903381\C,-4.3577888453,2.2514028915,1.783234892\H,-5.1908133806,1.570900666,1.5717479204\H,-4.6362847902,3.0007395635,2.5282179221\H,-4.0219653129,2.7276397353,0.853469177\H,-0.4451782889,-1.4762297926,0.8886591278\O,-3.0759450988,-2.321172757,-0.4527998715\O,-1.8989870591,-2.2454649694,-1.0184368767\O,-1.9425277257,-1.4591985147,2.5092938661\H,-3.2114442764,-1.4418370076,-0.0057555119\H,-1.3453576575,0.1600873709,-0.7044662677\Version=ES64L-G09RevE.01\HF=-878.6165998\S2=1.005684\S2-1=0.\S2A=0.047631\RMSD=2.505e-09\RMSF=2.902e-06\Dipole=0.5143062,2.2906971,0.3530475\Quadrupole=2.5921799,-0.7557944,-1.8363855,-9.8218029,-3.2408927,-1.4097096\PG=C01 [X(C9H1607)]\@

alkoxy

1\1\GINC-R2861\FOpt\UM11\6-31+G(d,p)\C9H15O5(2)\ROOT\21-May-2016\0\#\m11/6-31+g(d,p) opt=(maxcyc=200) freq=noraman nosymm scf=(tight,maxcyc=200) int=ultrafine\pMA-O* (tertiary)\0,2\C,-0.2157895444,0.4278042144,-0.1450600278\C,-0.5076271317,-0.1137311582,1.2572760227\C,1.2340218308,0.1150289159,-0.556205274\C,-0.4002638726,1.9339797039,-0.1846640158\C,-2.0340560974,-0.2361381639,1.6152207096\H,-0.0564186217,0.544202288,2.0152514856\H,1.4580245283,0.5355332506,-1.5448570654\H,1.9404751993,0.537957176,0.1724270699\H,1.3884004745,-0.9709497144,-0.5992011538\O,-0.6830431839,2.3740572151,-1.4118021997\O,-0.2778510551,2.6722286066,0.7741286051\C,-2.1794845422,-0.8011865981,3.0342690301\C,-2.6495766713,1.1695402402,1.451695707\C,-0.9957598095,3.7699348195,-1.5036442136\H,-3.2394990169,-0.888933775,3.3033954511\H,-1.7242643914,-1.7988498067,3.0612878085\H,-1.687707058,-0.144687954,3.760725548\O,-2.5900729926,1.8730995444,2.5840139779\O,-3.0773589979,1.6025607997,0.4062616069\H,-1.8852493362,3.9766255914,-0.8931917963\H,-0.1524838968,4.3729926989,-1.1453977271\H,-1.1981088637,3.9634397257,-2.5603814598\C,-2.9662252528,3.2549540904,2.4650448127\H,-3.9903923506,3.3304246184,2.0800896302\H,-2.8930241051,3.6718049427,3.4730459749\H,-2.2675443218,3.7539785666,1.7814799885\H,-0.0874859431,-1.1234189632,1.3632568457\O,-2.5379837438,-1.0925065182,0.677149051\H,-0.9102022324,-0.0034473567,-0.878850392\Version=ES64L-G09RevE.01\HF=-727.7463902\S2=0.753175\S2-1=0.\S2A=0.750007\RMSD=3.310e-09\RMSF=1.218e-05\Dipole=0.6015902,0.4036438,0.460993\Quadrupole=-5.7547096,3.6955651,2.0591445,-5.1687309,-5.4006985,-2.0422078\PG=C01 [X(C9H15O5)]\@

TS3a

1\1\GINC-R2880\FTS\UM11\6-31+G(d,p)\C9H15O5(2)\ROOT\21-May-2016\0\#\m11/6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) freq=noraman nosymm scf=(tight,maxcyc=200) int=ultrafine\TS for C-Calpha fragmentation : pMA-O* (tertiary)\0,2\C,-0.1899091783,1.4637771855,0.2504781133\C,0.6585260487,0.5340073149,1.0573320186\C,-0.0599595692,2.9255418176,0.7355603898\C,-1.6453198218,1.0351322354,0.3035675681\C,1.2710753589,-1.0180496275,-0.2447309972\H,0.165542935,-0.0600535594,1.8318447417\H,-0.6917572754,3.579632097,0.1219482791\H,-0.3666395979,3.021279859,1.7859551085\H,0.9813306977,3.258432588,0.6432024947\O,-2.3673933732,1.6150274746,-0.6553589329\O,-2.1164328517,0.266747912,1.1193662863\C,2.1295344214,-1.8158620738,0.723127926\C,-0.1923951464,-1.4863365008,-0.4442350339\C,-3.7163064682,1.1440214521,-0.7745441288\H,2.3645117252,-2.782856743,0.2554832846\H,3.0672283236,-1.273082088,0.8876877306\H,1.6209518064,-2.0147085887,1.6722144472\O,-0.5532623033,-2.3988264068,0.4616120765\O,-0.91880103,-1.0636037784,-1.3131687601\H,-3.700043805,0.0693905061,-1.0008057191\H,-4.2629952961,1.3172136366,0.1604164478\H,-4.1588

714911,1.7074302786,-1.6001757414\C,-1.9161944339,-2.8505180075,0.3689
768787\H,-2.0972020833,-3.2722710522,-0.6273433629\H,-2.0297326682,-3.
6129805016,1.1441868293\H,-2.587304655,-2.0018351354,0.5479881885\H,1.
6808503929,0.8569717065,1.2602701804\O,1.7731032479,-0.3476594404,-1.1
58935856\H,0.1233760903,1.4121034395,-0.8055534575\\Version=ES64L-G09R
evE.01\HF=-727.7277698\S2=0.769659\S2-1=0.\S2A=0.75008\RMSD=8.604e-09\
RMSF=2.546e-06\Dipole=-0.5271791,-0.0180275,1.0604858\Quadrupole=2.712
3208,5.2623921,-7.9747129,0.2586198,5.8644982,-0.2403436\PG=C01 [X(C9H
15O5)]\@

CH₃COR¹

1\1\GINC-R252\FOpt\RM11\6-31+G(d,p)\C4H6O3\ROOT\14-Jun-2016\0\#\ m11/6
-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=noram
an\beta-scission acetone fragment\0,1\C,2.0060641523,-0.6023754205,0
.5725218394\C,3.1034142395,-0.8202357364,-0.4344266775\C,1.2405482053,
0.7502151299,0.521948278\H,3.8646598385,-0.035289537,-0.3326472952\H,3
.5447274612,-1.8081605053,-0.2742754568\H,2.6983637057,-0.7376039646,-
1.4517984962\O,1.7043526829,1.5384420935,-0.4576542015\O,0.3465079387,
1.0464187658,1.2694168255\C,1.0484813639,2.8122372132,-0.5732348478\H,
1.1644337048,3.3736931701,0.3617438963\H,1.5356234048,3.3270367562,-1.
4051471058\H,-0.0194141747,2.6612332631,-0.7723993164\O,1.6798044873,-
1.4007472079,1.4133345679\\Version=ES64L-G09RevE.01\State=1-A\HF=-381.
541641\RMSD=4.157e-09\RMSF=4.675e-06\Dipole=0.8012441,0.9546089,-1.434
9651\Quadrupole=0.1932227,1.8836778,-2.0769005,-1.7038983,2.5944171,1.
6269533\PG=C01 [X(C4H6O3)]\@

ROOH

1\1\GINC-R370\FOpt\RM11\6-31+G(d,p)\C5H10O4\ROOT\26-Jun-2016\0\#\ m11/
6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=nora
man\beta-scission C fragment peroxide\0,1\C,1.1423542882,0.179628594
5,-0.4161260145\C,1.4950468501,1.4217595982,0.4163884028\C,-0.24584058
43,-0.3205259562,-0.0701287286\H,0.7676429363,2.2233909055,0.243042490
9\H,1.4996895801,1.1764384294,1.4881063443\H,2.4950951108,1.7780434934
,0.1432379338\O,-1.1870968416,0.6060288165,-0.3118349034\O,-0.50443338
8,-1.416191653,0.3789724813\C,-2.5301802334,0.2099093744,-0.0007980329
\H,-2.8084263646,-0.6696400165,-0.5943218519\H,-2.610381862,-0.0379906
782,1.0647266773\H,-3.1608746718,1.0669059619,-0.2519920366\H,1.127981
0434,0.4574289961,-1.4815820533\C,2.1362730211,-0.9587489289,-0.212574
919\H,1.8519529992,-1.8528658408,-0.7865863235\H,2.2163937399,-1.23116
79795,0.8517589184\O,3.386489966,-0.4676402583,-0.676586362\O,4.304951
9693,-1.544069783,-0.4685140976\H,5.1255010913,-1.1379619755,-0.782431
5153\\Version=ES64L-G09RevE.01\State=1-A\HF=-497.1519022\RMSD=8.858e-0
9\RMSF=1.767e-05\Dipole=-0.2125938,0.8749904,-0.2394454\Quadrupole=7.9
839926,-6.0474309,-1.9365618,-1.010385,-0.9209857,1.7164985\PG=C01 [X(
C5H10O4)]\@

Poly(methyl methacrylate)

pMMA

1\1\GINC-R252\FOpt\UM11\6-31+G(d,p)\C11H20O4\ROOT\26-Oct-2015\0\#\um11
/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=norama
n\MMA\0,1\C,-0.3072262122,1.3073978414,-0.4280748641\C,-0.6618462686
, -0.2046396591,-0.530102277\H,-1.7604217242,-0.2754751532,-0.459130569
2\H,-0.3801817695,-0.5476886663,-1.537102697\C,-0.0676857113,-1.229177
7058,0.4725697793\C,1.4295462707,-1.3948709329,0.2056350599\C,1.204486
2958,1.4352031688,-0.2523512611\O,1.678232794,-1.8454850738,-1.0295062
937\O,1.5783916799,1.8875153942,0.948388598\C,3.0633844223,-1.88178452
04,-1.401717894\H,3.6173956561,-2.5408017293,-0.7218472693\H,3.4711122
763,-0.8640819477,-1.3538101326\H,3.0875856389,-2.2650748697,-2.425608
1423\C,2.9980060188,1.9421927758,1.1719479188\H,3.4658562785,2.5898337
936,0.4202845792\H,3.4115851331,0.9286070108,1.1060054372\H,3.12284840
11,2.353668913,2.177331776\O,2.3111460887,-1.1555260491,1.0063422372\O
,2.0045716741,1.130643323,-1.1163024674\C,-0.2638877517,-0.8513174109,
1.9427032745\H,0.341368826,0.0205459872,2.2179986516\H,0.0487869884,-1
.683479525,2.5879239285\H,-1.3257326705,-0.6393102322,2.1354041855\C,-
0.6585934288,1.9409875945,-1.7880867967\H,-0.4933255368,3.0275056684,-
1.7701797649\H,-1.7197689138,1.7598084237,-2.0129684624\H,-0.043401315
5,1.5062771522,-2.5854238152\C,-1.0933037114,2.0339757523,0.6717734474

\H,-0.871934856,3.1099017877,0.6499039745\H,-0.8646612756,1.6700224097
,1.6770651073\H,-2.1697752921,1.904021076,0.4864463599\C,-0.7471203588
,-2.5844763154,0.1894891446\H,-1.8139836033,-2.5175261717,0.4467196733
\H,-0.2990063637,-3.3821543095,0.7987419517\H,-0.6536576788,-2.8605188
002,-0.8685723777\Version=ES64L-G09RevD.01\State=1-A\HF=-731.8021133\
S2=0.\S2-1=0.\S2A=0.\RMSD=3.552e-09\RMSF=1.238e-05\Dipole=-0.5083127,0
.0458166,-0.0430329\Quadrupole=2.2718744,1.2231177,-3.494992,0.5038789
,-0.3757392,2.6177127\PG=C01 [X(C11H2004)]\@

int-1

1\1\GINC-R3405\FOpt\UM11\6-31+G(d,p)\C11H2007\ROOT\13-Jul-2015\0\#\um1
1/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noram
an #guess=read geom=allcheck\O3 + pMMA caged complex\0,1\C,-0.070650
1329,0.1114492142,1.146548455\C,-1.2359710904,-0.9009568704,0.96139299
15\H,-0.7801197995,-1.823337646,0.5675235179\H,-1.6373793255,-1.138174
9654,1.9583374464\C,-2.4499179166,-0.5623426953,0.0569101942\C,-3.3022
982985,0.5081000006,0.7410973269\C,-0.6788305024,1.4717181561,1.478290
278\O,-3.7876121926,0.0949948764,1.917887972\O,-0.495422562,2.39869109
14,0.5335881082\C,-4.4589118079,1.1004941844,2.6907006879\H,-5.3171565
539,1.4929694618,2.1313979385\H,-3.7515149436,1.9101929433,2.910855202
\H,-4.7835808797,0.6038830327,3.6093096406\C,-1.1316768345,3.664301311
4,0.7806156763\H,-0.7671003274,4.0834054887,1.7265176153\H,-2.21744287
36,3.5171363975,0.8277174036\H,-0.8572486265,4.3027613355,-0.063641098
1\O,-3.5262723198,1.6138461598,0.2911445671\O,-1.3024983368,1.69069650
73,2.4996982703\C,-2.0720759635,-0.0692381999,-1.3416624775\H,-1.61941
60308,0.9287595007,-1.3060780564\H,-2.9715454176,0.000995756,-1.968421
5908\H,-1.3715021551,-0.7757066638,-1.8104959694\C,0.7208349277,-0.351
0225342,2.385283202\H,1.5993797165,0.2881155616,2.551635962\H,1.072680
1937,-1.381333691,2.2259406441\H,0.0892011386,-0.3198834662,3.28173177
46\C,0.8836104885,0.1562323871,-0.0547246065\H,1.7488294151,0.79382177
38,0.1739091178\H,0.4169200221,0.5463748475,-0.9628537094\H,1.24866774
73,-0.861447137,-0.2558307725\C,-3.2969852266,-1.8455333387,-0.0576082
569\H,-2.7323765526,-2.6007736024,-0.6246988289\H,-4.2356041297,-1.651
0082848,-0.5954716477\H,-3.5407463286,-2.2502048179,0.9331401771\O,0.2
384789516,-3.9844236847,-0.5813277577\O,-0.085547571,-3.1502625809,-1.
4696456319\O,1.0408020984,-3.5722898093,0.2992862344\Version=ES64L-G0
9RevD.01\State=1-A\HF=-957.1410382\S2=0.382303\S2-1=0.\S2A=0.003278\RM
SD=3.427e-09\RMSF=6.707e-06\Dipole=0.2364465,-0.6354812,-0.1402863\Qua
drupole=0.0817798,3.9398297,-4.0216094,0.7044959,-3.0392769,1.8080639\
PG=C01 [X(C11H2007)]\@

TS1a

1\1\GINC-R3528\FTS\UM11\6-31+G(d,p)\C11H2007\ROOT\13-Jul-2015\0\#\um11
1/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcf,oeigen,maxcy
c=200) freq=noraman #guess=read geom=allcheck\TS for O3 H abstraction
of pMMA\0,1\C,2.0116924261,-0.9596487547,-0.0013544932\C,1.019799325
2,0.1095456049,0.4979278071\C,1.4783979455,-1.8106447319,-1.1640278746
\C,2.3350728338,-1.8811639901,1.189198925\C,3.301228134,-0.2090241745,
-0.3661441102\C,0.7156327628,1.4132363039,-0.2503161212\H,1.1824619916
,0.3246134511,1.5646779419\H,0.630534833,-2.4118609732,-0.8100041231\H
,1.1577095241,-1.2151285595,-2.0235009238\H,2.2623153832,-2.4986504297
,-1.5065659202\H,3.009082992,-2.6912273698,0.8784305568\H,2.8168507153
,-1.3150810091,1.9958465593\H,1.4040215805,-2.3311889804,1.5624335295\
O,3.551058023,-0.1705816781,-1.6750437596\O,4.0128253972,0.3264041617,
0.4605594337\C,-0.4874155252,2.0969464423,0.4343129385\C,0.4514849657,
1.2581665226,-1.749305205\C,1.9419950863,2.3257501833,-0.0613862956\C,
4.7092224408,0.5942246633,-2.0594920857\H,-0.6369477963,3.1033286872,0
.019545294\H,-1.3946335399,1.5062734595,0.250875763\H,-0.3286089341,2.
1855873695,1.5165674098\H,1.3393143256,0.8984704892,-2.2823882744\H,-0
.3910985246,0.572377129,-1.9139542202\H,0.1875569166,2.2359724629,-2.1
726975137\O,2.1813076975,2.5894247255,1.22579848\O,2.6228707518,2.7589
275012,-0.9663081486\H,5.6023787909,0.1756806108,-1.5799920853\H,4.770
1732862,0.5089328235,-3.1476317096\H,4.5686613257,1.6370632105,-1.7510
106001\C,3.3945026488,3.3129528352,1.4894564239\H,3.4320952798,3.44522
07401,2.5740358316\H,4.245626848,2.7173404946,1.1355547744\H,3.3714088
682,4.2812875674,0.9751259866\H,-0.0904276778,-0.5248589646,0.58759805
53\O,-1.1329812801,-1.2218576897,0.8340987137\O,-1.6877357028,-1.51801
45427,-0.3753068456\O,-2.3554341183,-0.5517955908,-0.8596141147\Versi

on=ES64L-G09RevD.01\State=1-A\HF=-957.1123427\S2=0.817272\S2-1=0.\S2A=0.053811\RMSD=5.833e-09\RMSF=9.397e-06\Dipole=0.8281425,0.0767482,0.0730534\Quadrupole=-4.1578814,2.8749512,1.2829302,-2.3871238,-2.0750676,3.5676653\PG=C01 [X(C11H2007)]\@

TS1b

1\1\GINC-R1312\FTS\UM11\6-31+G(d,p)\C11H2007\ROOT\06-Apr-2016\0\#\ uml1/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcfc,noeigen,maxcyc=200) freq=noraman # guess=read geom=allcheck\TS for O3 H abstraction of pMMA (pri-C)\0,1\C,-1.9639867239,0.4460168999,-0.6531559137\H,-2.4970865173,0.8688504911,0.2119890774\C,-1.5633575664,-1.0061676807,-0.2693528602\H,-1.0314842888,1.020903735,-0.7805192177\C,-2.8236219964,0.7132439509,-1.9211970696\C,-0.6324187058,-0.9158570433,0.9299234196\C,-0.9046701495,-1.8035920118,-1.3977506299\C,-2.8091297103,-1.7717728488,0.2181436078\C,-2.0110311678,0.6482710578,-3.2213850768\C,-3.4037685103,2.133469608,-1.7700268881\C,-4.0052825613,-0.2539968444,-1.9111928847\H,-0.1864336504,-1.8652071932,1.251620335\H,-0.9845702195,-0.2925128089,1.7593761705\H,-0.5074499628,-2.7501791775,-1.0071177194\H,-1.6361728625,-2.0473269953,-2.1768278513\H,-0.070025193,-1.2311657209,-1.8240616629\O,-3.2571439408,-2.7648605156,-0.3115996767\O,-3.3481715253,-1.211993374,1.3051235565\H,-1.6131456025,-0.347599136,-3.432916647\H,-2.637855858,0.9431517481,-4.0739405286\H,-1.1707890668,1.3545033608,-3.1539105493\H,-3.9800248181,2.417544554,-2.6616115532\H,-4.0622402089,2.1902233658,-0.8944782791\H,-2.5817437531,2.8539213623,-1.6505263502\O,-4.8779474378,-0.228014261,-1.0636175776\O,-3.9861334428,-1.1522064024,-2.8987357901\C,-4.6074483715,-1.7669018729,1.7204603793\C,-5.0496173044,-2.1205136008,-2.8739061057\H,-4.9011041052,-1.204412844,2.6107368897\H,-5.3358619569,-1.6322712039,0.9111077179\H,-4.4880904752,-2.8330324515,1.9486946398\H,-4.89565171,-2.7506594063,-3.7540064482\H,-4.9803322913,-2.7077884166,-1.950407528\H,-6.0177513884,-1.6070653998,-2.9210485319\H,0.3893179377,-0.2499294553,0.4967559949\O,1.3883331869,0.3255327347,0.0200133034\O,2.407461623,-0.5497479849,0.2848897816\O,2.3234302953,-1.6068582186,-0.4125415335\Version=ES64L-G09RevE.01\State=1-A\HF=-957.1072345\S2=0.833148\S2-1=0.\S2A=0.054502\RMSD=4.085e-09\RMSF=1.990e-06\Dipole=-0.790117,0.2243426,0.2079689\Quadrupole=-7.1569894,-0.4498041,7.6067935,2.5205888,0.9332333,-1.6040001\PG=C01 [X(C11H2007)]\@

int-2 (rad)

1\1\GINC-R220\FOpt\UM11\6-31+G(d,p)\C11H1904(2)\ROOT\10-Jun-2016\0\#\ uml1/6-31+g(d,p) opt=maxcyc=200 scf=(tight,maxcyc=200) freq=noraman int=ultrafine\pMMA-C* (secondary)\0,2\C,2.1985228218,-0.7422422822,-0.2716054413\C,1.0827157019,0.2699232843,-0.286250761\C,1.8024834062,-1.894731989,0.6793093033\C,2.4812374769,-1.3149199073,-1.6783818466\C,3.4619552583,-0.1296474692,0.3371668367\C,1.0659170323,1.6278944118,-0.9521873299\H,0.0989947352,-0.0892688306,0.0288117505\H,2.6098078157,-2.6377672697,0.7397215549\H,1.5906575789,-1.5119119748,1.6866368847\H,0.9025630445,-2.3938590025,0.2927385666\H,1.5369930617,-1.6522935822,-2.1294114258\H,2.9434396171,-0.5547445815,-2.3193567804\H,3.1652360939,-2.1706982484,-1.6081903367\O,3.4633358485,0.7203847704,1.2054537426\O,4.5862044533,-0.67109642,-0.145071905\C,0.0453973382,2.5184724826,-0.2262507635\C,0.6600470227,1.4905917957,-2.4427613225\C,2.4701675907,2.2303595898,-0.9198293607\C,5.8002134377,-0.0756078659,0.3251362994\H,0.3047970679,2.6289100733,0.8331445595\H,0.0040807702,3.5173956674,-0.6805870958\H,-0.9508597008,2.0599723939,-0.3035273035\H,1.4118551661,0.9264967959,-3.0053154535\H,-0.3065411505,0.9728492598,-2.5118403303\H,0.5541908162,2.4853911838,-2.9003569711\O,3.4033836125,1.7856890758,-1.563485687\O,2.5888253695,3.2831612519,-0.1117963361\H,5.8346411995,0.9721867446,-0.0026879361\H,5.8483623235,-0.1209289519,1.4200430314\H,6.6131651765,-0.6484404252,-0.1296162948\C,3.9243765508,3.7715635768,0.0713870426\H,4.3734665743,4.0173568755,-0.8985954117\H,3.8336438386,4.6608768148,0.7011454129\H,4.5166960502,2.9962667526,0.5745361082\Version=ES64L-G09RevE.01\State=2-A\HF=-731.1330705\S2=0.753512\S2-1=0.\S2A=0.75001\RMSD=7.391e-10\RMSF=3.870e-06\Dipole=-0.0151052,-0.0574502,-0.0664966\Quadrupole=4.7795854,2.1262132,-6.9057986,1.6932959,3.066112,-0.6980372\PG=C01 [X(C11H1904)]\@

hydrotrioxide

1\1\GINC-R191\FOpt\UM11\6-31+G(d,p)\C11H2007\ROOT\05-Apr-2016\0\#\ um1
1/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noram
an\Intm 2 'zwitferionic' - secondary H abstr.\0,1\C,0.702465898,-1.4
890004375,0.0115622707\C,0.8938970273,0.0524932612,-0.0830950283\O,-0.
3222313684,0.7793421928,0.1550060651\O,-1.1868180212,0.7171654931,-0.9
61372167\O,-2.2685271928,-0.1040438946,-0.6089373183\H,-2.8698998526,0
.5171531426,-0.1664023001\C,1.7022719374,0.6810370736,-1.2710791491\H,
1.4530917038,0.3304097865,0.8261352842\C,-0.1855086205,-1.782777716,1.
2454118236\H,-1.2166766619,-1.4804749887,1.0365944517\H,-0.1688801618,
-2.8603587004,1.4618356176\H,0.1803172889,-1.2402503133,2.1279454821\C
,0.1189424726,-2.1830610149,-1.2265166078\H,0.8687873685,-2.2983373724
, -2.015328477\H,-0.217756662,-3.1905216113,-0.9484787418\H,-0.74271201
61,-1.6272598923,-1.6137534274\C,1.2455077065,0.3511871028,-2.70396486
21\H,1.767531195,1.0296899193,-3.3942345213\H,1.5065653063,-0.66904776
96,-2.9933264893\H,0.1687749661,0.5048599011,-2.8232910788\C,1.6815138
848,2.2083752192,-1.0787730966\H,1.9051022431,2.4921477503,-0.04314516
59\H,2.4245797477,2.6802303168,-1.735358611\H,0.6877461035,2.593432259
2,-1.3413299082\C,2.0673071578,-2.0698264665,0.3928477733\O,2.81417814
99,-1.5508075809,1.202373285\O,2.3399712298,-3.2322102265,-0.197251934
5\C,3.1262746613,0.139330999,-1.1006040823\O,3.5457992631,-0.862774888
8,-1.646982677\O,3.8555277892,0.8539233476,-0.2409555278\C,3.651145810
6,-3.753685188,0.0597215069\H,3.7033791785,-4.7070865314,-0.4729156081
\H,4.3944865626,-3.0461154982,-0.3316469596\H,3.7986642727,-3.89357103
02,1.1375345145\C,5.1420609602,0.3055702508,0.0824454467\H,5.738173925
8,0.188034639,-0.8308827124\H,5.6073856216,1.0213302433,0.7656260943\H
,5.0015611248,-0.6675017769,0.569586836\Version=ES64L-G09RevE.01\Stat
e=1-A\HF=-957.2217998\S2=0.\S2-1=0.\S2A=0.\RMSD=7.660e-09\RMSF=1.784e-
06\Dipole=-0.1240123,0.0633208,0.2388258\Quadrupole=7.2693938,0.239893
6,-7.5092874,-2.8317626,-1.0317964,-1.8745714\PG=C01 [X(C11H2007)]\@

TS2a

1\1\GINC-R2505\FTS\UM11\6-31+G(d,p)\C11H2007\ROOT\21-Aug-2015\0\#\um11
/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcf, noeigen,maxcy
c=200) freq #guess=read geom=allcheck\TS for for peroxy radical addi
tion to *OpMMA\0,1\C,-0.7404545144,1.6917579256,0.2492832784\C,-1.321
1007136,0.2366766224,0.2038876773\O,-0.500983062,-0.6053746461,-0.5198
354619\O,-0.7173592757,-0.3465863713,-2.4633151213\O,-0.8697205663,-1.
575661859,-2.9264448089\H,0.032568181,-1.9171073119,-3.0612545067\C,-2
.8508409247,0.018897171,-0.0782542565\H,-1.1731409112,-0.1729164191,1.
2305874052\C,-3.4288238364,0.8097267302,-1.2576571434\H,-2.885122361,0
.5694846818,-2.1776226455\H,-3.4022762216,1.8901370879,-1.0741418172\H
, -4.4833879673,0.5302643182,-1.383995838\C,-3.0789286922,-1.4898018295
, -0.2966002662\H,-2.643287515,-1.7904400547,-1.2564773051\H,-4.1566508
244,-1.7051744812,-0.3122553381\H,-2.6131680822,-2.0819318843,0.501556
6962\C,-0.5120174824,2.2953513236,-1.1410128641\H,0.2474239287,1.69915
32141,-1.6627843804\H,-0.136598042,3.3222277011,-1.0383308594\H,-1.417
0049258,2.3264108728,-1.754736084\C,0.6125047971,1.6120558204,0.982742
8407\H,1.2625394422,0.9023558676,0.4549250536\H,0.4748682124,1.2809487
508,2.0199806265\H,1.102533271,2.5956106309,0.9923757412\C,-1.67277244
4,2.5210274031,1.1279952448\C,-3.6317521086,0.4163164191,1.1800939305\
O,-3.2584925767,-0.2876316779,2.2561760016\O,-2.320476841,3.493732286,
0.484433425\C,-3.2606375221,4.2375722375,1.2803094242\H,-2.7400140952,
4.7084495626,2.123164712\H,-4.0350231371,3.5551079897,1.6512500975\H,-
3.6841219423,4.990280948,0.6098515014\C,-3.8536772549,0.1258229856,3.4
947994559\H,-3.5816636397,1.1713536892,3.6873746119\H,-3.4395207355,-0
.5355384313,4.2608539033\H,-4.9445481948,0.0264762644,3.4372338917\O,-
4.5086021071,1.2548568802,1.216872487\O,-1.8242693153,2.3041095824,2.3
159706906\Version=ES64L-G09RevD.01\State=1-A\HF=-957.1884329\S2=0.684
177\S2-1=0.\S2A=0.015873\RMSD=9.447e-09\RMSF=3.264e-06\Dipole=0.612396
9,-0.2984613,-0.3195714\Quadrupole=-2.9756334,2.959622,0.0160114,-2.85
81794,-6.1387364,2.6729475\PG=C01 [X(C11H2007)]\@

alkoxy1

1\1\GINC-R2507\FOpt\UM11\6-31+G(d,p)\C11H19O5(2)\ROOT\21-May-2016\0\#\#
m11/6-31+g(d,p) opt=(maxcyc=200) freq=noraman nosymm scf=(tight,maxcy
c=200) int=ultrafine\pMMA-O* (secondary)\0,2\C,-0.0287676919,-1.4772
043972,0.5875436767\C,-0.7235228571,-0.0676808475,0.6956643447\O,-2.05
42656849,-0.2381254307,0.9353376167\C,-0.4730758532,1.0250975985,-0.40

19426121\H,-0.341794866,0.3862483208,1.6435372228\C,-0.0666280204,-2.0
964016755,1.9960369771\H,-1.1086695216,-2.1355653494,2.3401324809\H,0.
3335193729,-3.1193620599,1.9777976918\H,0.5307657504,-1.5020261775,2.6
99008981\C,-0.7656888218,-2.4055232347,-0.3869207666\H,-1.8139179967,-
2.489560073,-0.0699909471\H,-0.7310266956,-2.0592937564,-1.4233038137\
H,-0.3138570439,-3.4060054958,-0.3555220143\C,-0.7587825358,0.52468630
35,-1.819099654\H,-0.7266534437,1.3688924099,-2.5204995391\H,-0.010155
6741,-0.205251389,-2.1490710116\H,-1.7618528704,0.0758248943,-1.856289
3965\C,-1.3783707205,2.2291129536,-0.0758951358\H,-1.2541951857,2.5500
947446,0.9664164305\H,-1.1297086418,3.0738176461,-0.7333122418\H,-2.42
67296613,1.9524358806,-0.2357012371\C,1.4362751464,-1.2601005393,0.221
209716\O,2.2379572535,-0.7413895456,0.9748766519\O,1.7598258516,-1.674
7913292,-1.0047804388\C,0.9744345057,1.5063797694,-0.315493281\O,1.782
699008,1.4497038663,-1.2192963954\O,1.257970424,2.0283868415,0.8834609
294\C,3.120556972,-1.4271065547,-1.4018782368\H,3.2193123743,-1.859446
0784,-2.401191802\H,3.297193907,-0.3447589371,-1.4203218205\H,3.805193
9964,-1.9094676782,-0.693636183\C,2.6322462377,2.3910814746,1.08742141
4\H,2.9330829502,3.1428854306,0.3476166102\H,2.6866861449,2.7949533163
,2.1020041286\H,3.2546878914,1.4928960982,0.9877206548\\Version=ES64L-
G09RevE.01\HF=-806.328349\S2=0.753269\S2-1=0.\S2A=0.750007\RMSD=7.637e
-09\RMSF=5.677e-06\Dipole=0.29876,-0.083914,-0.044394\Quadrupole=-1.47
42133,3.3494111,-1.8751978,-0.7099978,1.0053481,2.8109175\PG=C01 [X(C1
1H1905)]\@

TS3a

1\1\GINC-R1293\FTS\UM11\6-31+G(d,p)\C11H1905(2)\ROOT\22-May-2016\0\#\#
m11/6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) freq=noraman nosymm
scf=(tight,maxcyc=200) int=ultrafine\\TS for C-Calpha fragmentation :
pMMA-O* (secondary)\O,2\C,0.4895188596,1.2616826384,0.6966756972\C,0.
6877469574,-0.2548113882,0.9947795207\O,1.8774532656,-0.6620789214,1.
1193324949\C,0.0658647834,-1.4498550934,-0.4126857593\H,-0.0898189979,
-0.6574415416,1.6833225508\C,0.6174433239,1.9176095981,2.0936493299\H,
1.6212323012,1.7141019182,2.4899236186\H,0.4801258622,3.0051693744,2.0
170972082\H,-0.1365163066,1.5184910134,2.7839997553\C,1.5657018801,1.8
280487431,-0.2282761741\H,2.5462072497,1.4907934363,0.130307608\H,1.44
13207729,1.5142836842,-1.2685646649\H,1.5347372014,2.9255841338,-0.206
4952463\C,0.6988219288,-0.993943475,-1.7002659523\H,0.5170949137,-1.76
3452881,-2.4676313928\H,0.2507742728,-0.0606633837,-2.0609159253\H,1.7
82003341,-0.8805982847,-1.5665293204\C,0.5175811599,-2.801881843,0.093
4137439\H,0.1995306698,-2.9691931091,1.1294063298\H,0.0643791129,-3.58
50182935,-0.5349293893\H,1.6082519906,-2.8787073804,0.037541784\C,-0.9
351857548,1.5051869958,0.2309054803\O,-1.9067171688,1.2183649818,0.907
0788717\O,-1.032570548,2.0605565794,-0.9779677277\C,-1.4373322709,-1.2
917842061,-0.4068382678\O,-2.0644037345,-0.8209362969,-1.3351995607\O,
-2.0044040611,-1.7566290079,0.706439146\C,-2.3728153995,2.2971277098,-
1.4444272933\H,-2.2644574152,2.7839377791,-2.4174203169\H,-2.897677868
,1.3392915299,-1.5372779047\H,-2.899423357,2.9478615532,-0.7354147218\
C,-3.4229789841,-1.5453954618,0.8072805352\H,-3.932271885,-2.044245968
7,-0.0262659745\H,-3.7196166957,-1.9800278424,1.7654667742\H,-3.622182
3999,-0.4668782903,0.7830671434\\Version=ES64L-G09RevE.01\HF=-806.3168
944\S2=0.769473\S2-1=0.\S2A=0.750097\RMSD=8.751e-09\RMSF=2.198e-06\Dip
ole=-0.6131714,0.0087846,-0.3405361\Polar=0.,0.,0.,0.,0.,0.\Quadrupole
=-1.7635451,4.3671155,-2.6035704,1.7376055,-2.508109,-0.4859609\PG=C01
[X(C11H1905)]\@

CH₃COR¹

1\1\GINC-R348\FOpt\RM11\6-31+G(d,p)\C6H10O3\ROOT\14-Jun-2016\0\#\# m11/
6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=nora
man\\beta-scission acetone fragment\\O,1\C,-1.6817896449,-0.4075446221
, -0.450628404\C,-0.5111037223,-1.3628950634,-0.7038990415\O,-0.4442046
274,-2.4659804046,-0.218501168\H,0.2640101939,-0.9812912461,-1.4057705
937\C,-2.4918260328,-0.3904339087,-1.7707581181\H,-2.8867034921,-1.395
0412567,-1.9717250955\H,-3.3375356885,0.3045429647,-1.6805794868\H,-1.
8634019432,-0.0703422987,-2.6119946399\C,-2.5296619143,-0.8713907396,0
.727379365\H,-2.8828409204,-1.892130375,0.5365308338\H,-1.9469708239,-
0.8828749355,1.6563549813\H,-3.3913410003,-0.2064857711,0.864471729\C,
-1.0760951054,0.9814675378,-0.2866859065\O,-0.2977464371,1.4623334473,
-1.0843648706\O,-1.4854135466,1.6254177669,0.8108609831\C,-0.938168817

4, 2.9419322912, 0.9868065983\H, -1.3734521058, 3.3238821318, 1.9138595347\H, 0.1545759885, 2.8841316802, 1.0588740212\H, -1.2083903601, 3.5751108014, 0.1330722782\Version=ES64L-G09RevE.01\State=1-A\HF=-460.124357\RMSD=4.413e-09\RMSF=4.757e-06\Dipole=-0.7158433, 1.0506167, 0.2071433\Quadrupole=0.5652413, -2.2661305, 1.7008892, 1.7364105, 2.1737955, 4.7771569\PG=C01 [X(C6H10O3)]\@

ROOH

1\1\GINC-R139\FOpt\RM11\6-31+G(d,p)\C5H10O4\ROOT\26-Jun-2016\0\#\ m11/6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=noraman\beta-scission C fragment peroxide\0,1\C, -1.7332927889, 0.7933881817, 0.3382017897\H, -1.5861000029, 0.9834549327, 1.4084432936\H, -1.3298096615, 1.6330108937, -0.2423303012\H, -2.8060832832, 0.6999487208, 0.1285724959\C, -1.5911069284, -1.7091944336, 0.7172064521\H, -1.1291701726, -2.6381006625, 0.3640076015\H, -1.3869385576, -1.5907716699, 1.7878345342\H, -2.6742906402, -1.7641203566, 0.5503182759\C, 0.4598321097, -0.3455246943, 0.257013019\O, 0.9207347594, -0.4070338054, 1.373578699\O, 1.2048667973, -0.0684377207, -0.8273773381\C, 2.597819695, 0.1652050835, -0.5596604151\H, 3.0450036724, -0.7272169631, -0.1053021519\H, 3.0558604993, 0.3867608094, -1.5272651779\H, 2.7062772999, 1.0115644269, 0.1288964689\C, -1.0349177933, -0.5122536523, -0.0475715523\O, -1.264268443, -0.6274456263, -1.4498723994\O, -0.6258233442, -1.8026678778, -1.9250938419\H, 0.2070502029, -1.4358740962, -2.2654462921\Version=ES64L-G09RevE.01\State=1-A\HF=-497.161439\RMSD=3.967e-09\RMSF=2.299e-05\Dipole=0.6655091, 0.4915352, -0.1245776\Quadrupole=4.8298733, -0.1499401, -4.6799332, -0.3666796, -6.587808, -0.5602304\PG=C01 [X(C5H10O4)]\@

Poly(vinyl chloride)

pVC

1\1\GINC-R277\FOpt\RM11\6-31+G(d,p)\C5H10Cl2\ROOT\13-Jun-2016\0\#\ m11/6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=noraman\poly-Vinylchloride\0,1\C, 1.1798485876, 0.3756978593, 0.264016635\C, -0.1130705674, -0.3740362867, 0.5850563509\H, 0.1418529266, -1.3022618385, 1.1218316082\H, -0.731397951, 0.2358230313, 1.2599744485\C, -0.9366663577, -0.7674377117, -0.6387682661\C, 2.0879624157, -0.3543510892, -0.7139689609\H, 3.0486944998, 0.1645830096, -0.8105692692\H, 1.6167162462, -0.3846707955, -1.7068552292\H, 2.2802264201, -1.3820655497, -0.374293254\C, -2.248305312, -1.4352732609, -0.2530238243\H, -2.039429164, -2.3440566983, 0.3293086051\H, -2.8252859381, -1.7128911781, -1.1429814688\H, -2.8565503851, -0.7583280738, 0.3612564042\H, -0.3552612467, -1.4239017198, -1.2982263859\H, 0.9488865399, 1.380808822, -0.1064629657\Cl, -1.292172912, 0.7032018606, -1.6491567774\Cl, 2.0652510879, 0.6407903393, 1.8276718296\Version=ES64L-G09RevE.01\State=1-A\HF=-1116.7796932\RMSD=2.690e-09\RMSF=9.425e-06\Dipole=-0.3132063, -0.8772413, -0.2739576\Quadrupole=0.0168682, 2.5639433, -2.5808115, 1.2411972, -4.4536459, 0.1970475\PG=C01 [X(C5H10Cl2)]\@

int-1

1\1\GINC-R405\FTS\UM11\6-31+G(d,p)\C5H10Cl2O3\ROOT\13-Jun-2016\0\#\ um11/6-31+G** opt=(ts,calcf, noeigen,maxcyc=200) scf=(tight,maxcyc=200) int=ultrafine freq=noraman # guess=read geom=allcheck\O3 + pVinylchloride caged complex\0,1\C, 1.053201135, 0.962687338, 0.7704926785\C, 0.6272128632, 0.3156324064, -0.5425490257\H, -0.4547131474, 0.4776838513, -0.6699028417\H, 1.1410601707, 0.8265428999, -1.3731862227\C, 0.9197097289, -1.1754871185, -0.6638075394\C, 0.6637287506, 2.4310057123, 0.8456804264\H, 1.0166775363, 2.8811214897, 1.7809262784\H, -0.4316549619, 2.5219870288, 0.8066106392\H, 1.0958301878, 2.9897699527, 0.0044179141\O, -2.7327961731, -0.5254567606, 1.5972567837\O, -1.9890868841, 0.459748466, 1.3415833115\O, -3.1480929381, -1.1760689489, 0.6049163371\H, 1.9853693896, -1.367821501, -0.491520671\H, 0.6376823537, 0.4059505021, 1.6190730601\C, 0.4655845922, -1.7442028118, -1.9991809808\H, -0.6133914865, -1.5884160863, -2.1350074758\H, 1.0001524238, -1.2350970227, -2.8138613782\H, 0.6741398146, -2.8186095131, -2.0617850538\Cl, 0.0725523635, -2.0767465366, 0.6761307968\Cl, 2.8577263511, 0.8108883425, 0.9567515434\Version=ES64L-G09RevE.01\State=1-A\HF=-1342.1213144\S2=0.376453\S2-1=0.\S2A=0.003135\RMSD=7.509e-09\RMSF=2.180e-04\Dipole=-0.5914317, 0.4315395, -0.6099071\Quadrupole=-2.8138883, -0.3632056, 3.1770939, -2.7357815, -3.4307372, 1.1222794\PG=C01 [X(C5H10Cl2O3)]\@

TS1b

```
1\1\GINC-R279\FTS\UM11\6-31+G(d,p)\C5H10Cl2O3\ROOT\13-Jun-2016\0\#\# um
11/6-31+G** opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200)
int=ultrafine freq=noraman # guess=read geom=allcheck\TS for O3 H abs
traction of pVinylchloride (pos. a)\0,1\C,0.8088287793,-1.1826323199,
0.7210595694\C,0.3680124416,0.2507015742,0.5255474646\C,0.8569755854,1
.0307816106,-0.6717155842\H,0.4504569141,0.8231797686,1.4625211201\C,0
.2064273314,2.3987403349,-0.7948557778\H,0.6359851339,2.9516611035,-1.
6379392903\H,-0.870589325,2.2682863346,-0.967741354\H,0.3572104945,2.9
847237378,0.1218200393\H,-0.9241490651,0.2230817643,0.4019199982\O,-2.
1684271479,0.1866274446,0.2965364659\O,-2.374966469,-0.6264117913,-0.7
833013722\O,-1.9501437498,-0.1060418162,-1.8580008621\H,0.7329194246,0
.4424814012,-1.5873733477\H,1.892076074,-1.1783555065,0.9132633567\C,0
.0599587794,-1.8741662641,1.853214965\H,0.2026718345,-1.3122799395,2.7
871300957\H,-1.0143245573,-1.9203155406,1.6310769183\H,0.4349920258,-2
.8938303681,1.9957661842\Cl,2.6613242373,1.2203802134,-0.4642246375\Cl
,0.6120834483,-2.1271110115,-0.8096119617\Version=ES64L-G09RevE.01\St
ate=1-A\HF=-1342.087885\S2=0.823295\S2-1=0.\S2A=0.056039\RMSD=8.303e-0
9\RMSF=2.180e-06\Dipole=0.1236462,0.2667565,1.0128755\Quadrupole=-4.99
45274,1.568842,3.4256854,-1.3768527,0.6370945,-2.5606166\PG=C01 [X(C5H
10Cl2O3)]\@
```

TS1a

```
1\1\GINC-R536\FTS\UM11\6-31+G(d,p)\C5H10Cl2O3\ROOT\13-Jun-2016\0\#\# um
11/6-31+G** opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200)
int=ultrafine freq=noraman # guess=read geom=allcheck\TS for O3 H abs
traction of pVinylchloride (pos. b)\0,1\C,1.7327047751,-0.7703843052,
0.162488391\C,0.6298432733,-0.5806104444,1.1984786135\C,-0.3970093796,
0.4886121649,0.8600490489\H,1.1133510937,-0.2903076268,2.1474373156\H,
0.1166506007,-1.5368886898,1.3783702875\O,-2.2511856007,-0.3080994874,
-0.6690563652\O,-1.9166348677,-0.1930530036,-1.9784591711\O,-1.7834158
582,1.0153938604,-2.3428627203\H,-1.2177140794,0.0055375984,-0.0036997
858\H,2.2699522015,0.1727224501,0.0000237452\C,0.0918323892,1.79206650
79,0.2706170577\H,0.7855681966,2.2829094206,0.9718063783\H,0.606272202
6,1.6062579198,-0.6816155906\H,-0.7530231198,2.4628904752,0.0789294922
\C,2.7049732712,-1.8693784508,0.5671996742\H,3.1814519985,-1.609303727
,1.5230651351\H,2.1761584937,-2.8241631969,0.6862162342\H,3.4864854554
,-1.9963598532,-0.1908477328\Cl,-1.5035714345,0.7369034434,2.221861992
6\Cl,0.9974797485,-1.1768881158,-1.4432338001\Version=ES64L-G09RevE.0
1\State=1-A\HF=-1342.0875144\S2=0.802486\S2-1=0.\S2A=0.050625\RMSD=6.2
36e-09\RMSF=1.788e-06\Dipole=1.6022247,0.0054933,1.0360491\Quadrupole=
1.4765215,1.8046624,-3.2811838,0.4492182,1.9605792,-0.6686301\PG=C01 [
X(C5H10Cl2O3)]\@
```

int-2 (rad)

```
1\1\GINC-R180\FOpt\UM11\6-31+G(d,p)\C5H9Cl2(2)\ROOT\13-Jun-2016\0\#\# m
11/6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=n
oraman\pVinylchloride-C* (tertiary)\0,2\C,1.7992171895,-0.8234943097
,0.2131450809\C,0.6879598232,-0.5922476971,1.2345269063\C,-0.289395880
2,0.4791915702,0.8603331066\H,1.1775416832,-0.3321037659,2.1943871385\
H,0.1501027403,-1.5375851721,1.4052723455\H,2.3315935173,0.1141121762,
0.0072140139\C,0.0976705327,1.7266482175,0.1403407508\H,0.7255152553,2
.3835543215,0.7706467327\H,0.6616069671,1.4823659329,-0.7706240744\H,-
0.7927324642,2.2953117035,-0.1519744416\C,2.7776569627,-1.8968649789,0
.6685141085\H,3.2557982824,-1.586626796,1.6084856609\H,2.2521300158,-2
.8459028742,0.8387775305\H,3.5572639305,-2.0611146635,-0.0844689534\Cl
,-1.6732595458,0.5853168513,1.906019627\Cl,1.0749403502,-1.3125155658,
-1.3774273326\Version=ES64L-G09RevE.01\State=2-A\HF=-1116.1181523\S2=
0.753624\S2-1=0.\S2A=0.750011\RMSD=3.581e-09\RMSF=7.172e-06\Dipole=0.9
810945,0.2289448,0.4503526\Quadrupole=0.6680838,1.7591687,-2.4272525,0
.1721415,2.3669303,-2.5549499\PG=C01 [X(C5H9Cl2)]\@
```

hydrotrioxide

```
1\1\GINC-R215\FOpt\RM11\6-31+G(d,p)\C5H10Cl2O3\ROOT\13-Jun-2016\0\#\# m
11/6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq=n
oraman\Intm 2 'zwitterionic' - OOH pos. b)\0,1\C,2.1106300381,-0.1570
699437,-0.0012392716\C,0.7501562564,-0.3423189023,-0.6732326477\C,-0.4
06723984,-0.7789309999,0.2339135821\H,0.8787261541,-1.121332306,-1.437
```

9596363\H,0.4499453903,0.5813915644,-1.1891883372\O,-1.2319005245,0.18
08233839,2.9827875587\O,-1.8910696604,0.1668081859,1.7442619616\O,-0.9
162179202,0.4264334015,0.7624344815\H,-1.1537488682,1.1305778694,3.173
9079376\H,2.4024941723,-1.0768092079,0.5208460093\C,-0.0395199538,-1.8
035945436,1.2933072047\H,0.4187492907,-2.6733759625,0.8055409057\H,0.6
590364803,-1.3542627273,2.0107255517\H,-0.9351519471,-2.128541822,1.83
27763423\C,3.1731839559,0.2228305396,-1.0249419111\H,3.2559302729,-0.5
667603196,-1.7852755447\H,2.9055259386,1.1637059424,-1.5237238848\H,4.
1494010092,0.3502250125,-0.542886569\C1,2.0644390305,1.1142375136,1.29
10901743\C1,-1.7027908111,-1.5106278885,-0.8386982969\Version=ES64L-G
09RevE.01\State=1-A\HF=-1342.20513\RMSD=6.370e-09\RMSF=1.805e-05\Dipol
e=1.1239581,-0.1219638,-0.1439809\Quadrupole=-2.7680403,0.9948372,1.77
32031,-4.1482893,-4.5086908,1.5020386\PG=C01 [X(C5H10C12O3)]\@

TS2a

1\1\GINC-R542\FTS\UM11\6-31+G(d,p)\C5H10C12O3\ROOT\13-Jun-2016\0\#\# um
11/6-31+G** opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200)
int=ultrafine freq=noraman # guess=read geom=allcheck\TS for for pero
xyl radical addition to *OpVinylchloride pos. b\0,1\C,-1.5216697221,-
0.3511963442,-0.0251417701\C,-0.4930193994,0.4351621874,-0.853839979\C
,0.5546437277,1.1049632618,0.0552453461\H,-0.9913619137,1.2210451454,-
1.4386901648\H,0.0353578335,-0.220258409,-1.5531290612\O,1.537194836,-
2.4242934638,0.4791773266\O,1.7711508577,-1.3460615556,-0.2235388013\O
,1.1324558145,0.2503219773,0.9292845076\H,0.5914497929,-2.6383480503,0
.3159152827\H,-1.2234795191,-0.3655698472,1.0301704518\C,-0.046454084,
2.2260106215,0.9274562033\H,-0.4764509394,2.9878851102,0.2661835818\H,
-0.8261900048,1.8124783989,1.5808736492\H,0.7383513562,2.6780930905,1.
5428254104\C,-2.9444851693,0.1629664931,-0.1799274222\H,-2.9785485157,
1.2151152075,0.1401754637\H,-3.261502467,0.1114612817,-1.2298676279\H,
-3.6484279521,-0.4138466686,0.4313206935\C1,-1.4908200994,-2.121374742
4,-0.4916806649\C1,1.8054898977,1.8775508057,-1.0502136953\Version=ES
64L-G09RevE.01\State=1-A\HF=-1342.1701939\S2=0.780531\S2-1=0.\S2A=0.02
1237\RMSD=4.765e-09\RMSF=5.096e-06\Dipole=-1.8717541,0.4870226,0.28336
97\Quadrupole=-2.8533272,2.1231161,0.7302111,-2.3403642,-1.1113183,1.8
395145\PG=C01 [X(C5H10C12O3)]\@

alkoxyl

1\1\GINC-R153\FOpt\UM11\6-31+G(d,p)\C5H9C12O1(2)\ROOT\14-Jun-2016\0\#\#
m11/6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq
=noraman\pVinylchloride-O* (tertiary)\0,2\C,1.3049409401,-0.87413179
86,0.1042337484\C,0.0173654996,-0.548887311,-0.6673460433\C,-1.2200068
543,-0.4089848056,0.2612250692\H,-0.2080873828,-1.3307280086,-1.405584
9254\H,0.1153739849,0.4017402469,-1.2042680251\O,-1.0433702543,0.63132
04236,1.0776928575\H,1.2400107574,-0.4671284068,1.1213025404\C,-1.5144
343996,-1.6478019029,1.1319270399\H,-1.6352030932,-2.5173878395,0.4750
058903\H,-0.6880850712,-1.8065544043,1.8355673011\H,-2.4415082955,-1.4
84318224,1.6912650792\C,1.6442593723,-2.3601062606,0.1209335801\H,0.82
45615367,-2.9388716199,0.5673716729\H,1.802453253,-2.72001495,-0.90439
27602\H,2.5577502956,-2.54553904,0.698081321\C1,2.6932670803,0.0134176
479,-0.655779679\C1,-2.6786623693,-0.1663597467,-0.8510786671\Version=
ES64L-G09RevE.01\State=2-A\HF=-1191.303821\S2=0.753121\S2-1=0.\S2A=0.
750007\RMSD=4.045e-09\RMSF=2.508e-05\Dipole=0.1051601,-1.3112458,0.478
9033\Quadrupole=-4.8504629,2.1979615,2.6525014,0.6172471,-0.4711491,-1.
.8578773\PG=C01 [X(C5H9C12O1)]\@

acetone+Cl*

1\1\GINC-R143\FOpt\UM11\6-31+G(d,p)\C5H9C12O1(2)\ROOT\27-Jun-2016\0\#\#
m11/6-31+G** opt=maxcyc=200 scf=(tight,maxcyc=200) int=ultrafine freq
=noraman\pVinylchloride=O---Cl* cpx (tertiary)\0,2\C,-1.4302426424,0
.0616470639,0.1039782462\C,-0.1099461051,-0.0217064478,-0.6731717522\C
,0.990837834,0.6555627386,0.1238539697\H,-0.2275696033,0.4552354146,-1
.6559921185\H,0.1648911336,-1.076476562,-0.8128266468\O,1.344212054,0.
2201594652,1.2085948281\H,-1.3299720334,-0.4926192856,1.0440962666\C,1
.6156809689,1.9013989948,-0.4472842542\H,2.0970659812,1.6547020522,-1.
4046949025\H,0.8281243249,2.638284688,-0.6633951735\H,2.3503457907,2.3
158104214,0.2491287936\C,-1.880824003,1.4929824342,0.3602725687\H,-1.1
588599316,2.0009645356,1.0176331623\H,-1.9622595142,2.0504129966,-0.58
3821456\H,-2.8581211288,1.5083371153,0.8561922138\C1,-2.6967611415,-0.

8105973229,-0.8481835902\C1,0.7363584558,-2.132113542,1.8009729947\\Version=ES64L-G09RevE.01\State=2-A\HF=-1191.3152589\S2=0.752801\S2-1=0.\S2A=0.750005\RMSD=6.438e-09\RMSF=2.409e-05\Dipole=0.2609203,1.519989,-0.9283362\Quadrupole=-1.9506129,3.1108023,-1.1601894,1.6129496,-6.2898997,-0.2826604\PG=C01 [X(C5H9C12O1)]\@

Cumene

cumene

1\1\GINC-R168\FOpt\RM11\6-31+G(d,p)\C9H12\ROOT\11-Jun-2016\0\#\# m11/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noraman\\Phenyl group\\0,1\C,2.0994250246,-0.0925519726,0.461455942\C,3.1992977742,0.4181462153,-0.4810207383\H,2.9650591147,0.1627715129,-1.5252695331\H,3.3049108392,1.5093743238,-0.4170801736\C,1.9736550817,-1.6203125775,0.3670762109\H,1.1952079884,-1.99930877,1.0426539672\H,2.9262067324,-2.1044806545,0.6252913933\H,1.7095300002,-1.9255453598,-0.6564523415\H,2.3856200545,0.1647909135,1.493576864\C,0.7703656442,0.5894198855,0.1798830418\C,0.1445792756,1.370854151,1.1530202988\C,0.1425702792,0.4494349152,-1.0630626255\C,-1.0749587304,1.9978140535,0.8976349556\H,0.6223186069,1.4897798725,2.1286987363\C,-1.0744050655,1.0723494037,-1.3244904709\H,0.6139126287,-0.157573883,-1.8403833464\C,-1.6888604267,1.8503712726,-0.343133226\H,-1.5460366934,2.6039408647,1.6732123733\H,-1.547407493,0.9504897812,-2.3003768376\H,-2.6426151206,2.3390156886,-0.5468926187\H,4.1666174851,-0.0414976364,-0.2330898715\\Version=ES64L-G09RevE.01\State=1-A\HF=-349.9700537\RMSD=8.407e-09\RMSF=3.078e-06\Dipole=0.1277633,-0.0601209,0.040153\Quadrupole=0.6261297,-2.0111696,1.3850399,-2.3035019,1.1996707,1.5351803\PG=C01 [X(C9H12)]\@

TS(1,3dipolar)

1\1\GINC-R2407\FTS\RM11\6-31+G(d,p)\C9H12O3\ROOT\12-Jun-2016\0\#\# m11/6-31+g(d,p) opt=(ts,calcfc,noeigen,maxcyc=200) scf=(tight,maxcyc=200) freq=noraman int=ultrafine\\TS for O3 1,3 dipolar cycloaddition\\0,1\C,0.9486391198,-0.2109664735,0.4972583036\C,2.2135601277,0.2926695285,0.9294057263\H,3.0156126414,0.3989182247,0.1995294196\O,1.2088147985,-2.2350053197,0.8587089627\O,2.4865915022,-2.2768765711,0.7199115742\O,3.0578273235,-1.4959696679,1.5660475948\H,0.8126090736,-0.4572379859,-0.5571226597\C,2.2903836622,1.0135509477,2.160761968\H,3.2443754692,1.4396070971,2.4706269402\C,1.1846997858,1.1078312819,2.9507521613\H,1.2435447054,1.6163434826,3.9143171547\C,-0.0738645548,0.5747852487,2.5280771631\H,-0.9333969304,0.6821477959,3.1909581961\C,-0.2202755527,-0.0301428669,1.3122794645\C,-1.5338008429,-0.5702826193,0.7771709927\H,-1.3190099088,-1.5833980831,0.3963326529\C,-2.6261772334,-0.6819338793,1.8417856835\H,-2.2932525582,-1.277720541,2.7025822723\H,-3.5177108796,-1.162343322,1.4168624699\H,-2.9299602362,0.3122933149,2.2033288546\C,-2.0253326001,0.2906073503,-0.4002741714\H,-1.2739167187,0.3684188378,-1.1979614885\H,-2.2561857655,1.3083727574,-0.0532951558\H,-2.937774428,-0.1386685378,-0.8370440795\\Version=ES64L-G09RevE.01\State=1-A\HF=-575.2851897\RMSD=5.974e-09\RMSF=6.323e-06\Dipole=-0.5263133,0.8383454,-0.2171081\Quadrupole=0.8301403,-3.1991152,2.368975,3.4202488,-1.2233578,1.9372105\PG=C01 [X(C9H12O3)]\@

primary ozonide

1\1\GINC-R2546\FOpt\RM11\6-31+G(d,p)\C9H12O3\ROOT\12-Jun-2016\0\#\# m11/6-31+g(d,p) opt=(maxcyc=200) scf=(tight,maxcyc=200) freq=noraman int=ultrafine\\primary ozonide\\0,1\C,0.1918227128,-0.7233762972,1.3640607645\C,-0.418382268,-1.8140639333,0.4652794476\H,0.3534788989,-2.4458577468,0.0054631695\H,-1.0683979907,-2.469921633,1.0598549713\C,-0.8985566946,-0.0154335395,2.1682384228\H,-0.4780936217,0.7216796642,2.8657994743\H,-1.4657471069,-0.7486098225,2.7568458765\H,-1.6071188147,0.5006305913,1.5023605377\O,4.2099274514,-1.1796648326,0.1189427416\O,4.3384073005,0.2153390623,-0.015857255\O,2.8658915621,-1.3147985045,0.5613374273\H,0.8752663671,-1.224582075,2.0708497992\C,1.0558970037,0.2292564914,0.561610871\C,2.1199146108,-0.4208724291,-0.2916209436\C,0.9380856888,1.5639732372,0.565147663\C,3.2207164111,0.5103081177,-0.8693573014\H,1.6595035983,-1.00237594,-1.1064244602\C,1.8606884659,2.4419699609,-0.1685681662\H,0.1509531302,2.0403988966,1.1501714796\C,2.9302051608,1.9771408879,-0.8206482132\H,3.479199568,0.1831704484,-1.887833833\H,1.665379553,3.5156323777,-0.1477762162\H,3.6254078599,2.6445852012,-1.3

299570546\H,-1.0283178066,-1.3653117034,-0.3333739725\\Version=ES64L-G
09RevE.01\State=1-A\HF=-575.3585232\RMSD=9.423e-09\RMSF=6.980e-06\Dipo
le=-1.1847605,0.6066981,-0.5431698\Quadrupole=-4.0851995,2.1638315,1.9
213681,2.3775994,-3.7054813,-0.3882882\PG=C01 [X(C9H12O3)]\@

TS1(sp²) step-wise

1\1\GINC-R2938\FTS\UM11\6-31+G(d,p)\C9H12O3\ROOT\15-Aug-2016\0\#\# um11
/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcfc,noeigen,maxcy
c=200) freq=noraman # guess=read geom=allcheck iop(1/8=1)\TS for O3 C
(sp2)-H abstraction on Cumene phenyl\0,1\C,-0.0043234054,2.6746702991
,-1.0506936983\H,0.8670689161,3.201264889,-0.6337597859\C,-0.440023038
6,1.5198608255,-0.1383610384\H,0.263216546,2.3158569147,-2.0534798237\
O,-1.8925778358,-1.5332425774,-1.1065680383\O,-2.4143362952,-1.8874067
646,0.1242464498\O,-2.4969123887,-0.891027721,0.903824777\H,-1.3325805
596,1.0457848004,-0.5704477665\H,-0.8179413111,3.4062429211,-1.1499664
221\C,-0.8043254372,2.0300517784,1.2629621814\H,0.0607405811,2.5174631
076,1.7378243024\H,-1.6159598726,2.7681229574,1.2004771813\H,-1.134089
6181,1.2060593937,1.9089697625\C,0.6388703896,0.4535282325,-0.04752860
77\C,0.4265847734,-0.8700361558,-0.3795916965\C,1.9382117963,0.7423035
453,0.4016880816\C,1.3423234459,-1.9004247187,-0.3030879718\H,-0.79005
80679,-1.1974292546,-0.8361947397\C,2.910624019,-0.2494862733,0.495463
7232\H,2.1814051139,1.7691621031,0.6862182789\C,2.6224171108,-1.569487
6277,0.1459658889\H,1.0800951119,-2.9209524035,-0.5832887035\H,3.90937
05166,0.00970914,0.8492253138\H,3.3877865096,-2.3427884112,0.221623351
8\\Version=ES64L-G09RevE.01\State=1-A\HF=-575.2695955\S2=0.874184\S2-1
=0.\S2A=0.075546\RMSD=8.135e-09\RMSF=3.256e-06\Dipole=1.1453538,0.3160
73,0.0350299\Quadrupole=0.2034047,3.472453,-3.6758577,-3.1612211,1.568
3667,0.4763069\PG=C01 [X(C9H12O3)]\@

TS1(sp²) concerted

1\1\GINC-R2830\FTS\UM11\6-31+G(d,p)\C9H12O3\ROOT\13-Aug-2016\0\#\# um11
/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcfc,noeigen,maxcy
c=200) freq=noraman # guess=read geom=allcheck\TS for O3 C(sp2)-H abs
traction on Cumene phenyl\0,1\C,5.0418947699,-1.1227795741,2.55843420
82\C,4.0584909699,-0.3541833272,1.6735770215\H,4.7989788064,-0.9996699
429,3.6247847414\H,5.0546456251,-2.1963764486,2.3245763485\O,2.3333899
942,-0.6790615187,-0.8715533792\O,3.0839516359,0.3817335207,-1.0853294
487\O,2.3565286794,1.4584120843,-0.9353385567\H,4.394012194,-0.4369987
173,0.6249955996\C,4.0661989103,1.1445155114,2.0330208704\H,3.69444533
28,1.2946846274,3.0571955661\H,5.0929912607,1.5313615198,1.9817762887\
H,3.4535979975,1.7375510717,1.3418301005\C,2.6513462572,-0.9052963333,
1.708986555\C,2.234687015,-1.8711508034,2.6281161116\C,1.6943605871,-0
.4144762667,0.7724516654\C,0.9255799503,-2.3418680398,2.6263929642\H,2
.9431850333,-2.2714139528,3.3527767422\C,0.3722217192,-0.9404862487,0.
7619729196\H,1.7614599941,0.6993233528,0.4685110171\C,-0.016021538,-1.
8760422246,1.6926942156\H,0.6302333843,-3.0993189004,3.3546984412\H,-0
.3143262184,-0.5805255917,-0.0059947854\H,-1.034111748,-2.2653289268,1
.6989626013\H,6.0567550877,-0.732525021,2.4070474021\\Version=ES64L-G0
9RevE.01\State=1-A\HF=-575.2705169\S2=0.\S2-1=0.\S2A=0.\RMSD=4.476e-09
\RMSF=9.285e-06\Dipole=-0.2548585,-1.0409052,1.4990338\Quadrupole=6.29
23744,-2.5870852,-3.7052892,2.4683087,0.3171443,0.5300762\PG=C01 [X(C9
H12O3)]\@

int-1

1\1\GINC-R234\FOpt\UM11\6-31+G(d,p)\C9H12O3\ROOT\29-Jun-2016\0\#\# um11
/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=norama
n # guess=read geom=allcheck\Cumene + O3 complex\0,1\C,0.3364091971,
-1.637774112,-1.4685593964\H,-0.1727575518,-2.5644574405,-1.163959859\
C,0.1722300495,-0.5538205767,-0.3927755992\H,-0.0946056992,-1.31554366
16,-2.4256935577\O,0.9728036694,2.3893819262,0.8080964826\O,2.10064482
61,1.8796315579,1.0438509901\O,2.7954697736,1.5770958295,0.037083871\H
0.6931462096,0.3514032809,-0.7460763736\H,1.3990481136,-1.8719564365,
-1.625127115\C,0.8128249078,-1.0078237302,0.9278807865\H,0.3822321197,
-1.9647093892,1.2576517565\H,1.8958931588,-1.157521912,0.8057112745\H,
0.6425494808,-0.2782862519,1.7325444507\C,-1.289293055,-0.1827593659,-
0.2026276485\C,-1.7517184729,1.0922256012,-0.5346410783\C,-2.206471903
1,-1.1138228834,0.2973859663\C,-3.094263066,1.4336713118,-0.3713283743
\H,-1.046010897,1.8279677889,-0.928082577\C,-3.5472925685,-0.778555274

4, 0.4631662998\H, -1.8669840625, -2.1191116416, 0.5603346523\C, -3.9964484
888, 0.4992596802, 0.1296202639\H, -3.4346031373, 2.4359514403, -0.63662644
54\H, -4.2470477959, -1.5186291274, 0.8550237614\H, -5.0468908081, 0.763174
3865, 0.2596904688\Version=ES64L-G09RevE.01\State=1-A\HF=-575.3090781\
S2=0.378759\S2-1=0.\S2A=0.003211\RMSD=7.292e-09\RMSF=7.430e-06\Dipole=
0.1742123, -0.0638968, 0.1706202\Quadrupole=1.2520279, 1.7733672, -3.02539
51, 0.3302136, 0.2281246, -1.1130509\PG=C01 [X(C9H12O3)]\@

TS1a

1\1\GINC-R158\FTS\UM11\6-31+G(d,p)\C9H12O3\ROOT\30-Jun-2016\0\#\ um11/
6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts, calcfc, noeigen, maxcyc
=200) freq=noraman # guess=read geom=allcheck\TS for O3 H-abstraction
on Cumene\0, 1\C, 0.7179049089, -0.6748072398, 1.5258171356\C, -0.1413543
029, 0.5501323578, 1.2648938095\H, 1.0850097789, -0.6696198666, 2.56493856\
H, 0.1633254603, -1.6073189861, 1.3594644368\O, -0.4979494752, 0.5163318767
, -1.2918317328\O, -0.0974095293, 1.7519819995, -1.6150144427\O, -0.9836984
484, 2.6388591034, -1.3973341083\H, -0.4244896496, 0.4665580289, 0.07166318
57\C, 0.6506113343, 1.8509274152, 1.3352273394\H, 1.0882073826, 1.951463600
8, 2.3410814182\H, 1.4753265446, 1.8470357894, 0.6077580848\H, 0.0219688049
, 2.7300201814, 1.1485711879\C, -1.4796973939, 0.5892173345, 1.9423630476\C
, -1.8196524053, -0.3106113339, 2.9594476548\C, -2.4232899459, 1.5523833147
, 1.5552401539\C, -3.0588446379, -0.2317964646, 3.592276015\H, -1.106479503
8, -1.0734411125, 3.2741950979\C, -3.6613000724, 1.6269701524, 2.1821745193
\H, -2.1875328001, 2.228765354, 0.7298635634\C, -3.9822472242, 0.7367287972
, 3.2074798808\H, -3.302484982, -0.9339492484, 4.3909374914\H, -4.384866895
2, 2.3779936724, 1.8622768372\H, -4.9540913876, 0.7940896766, 3.6995132643\
H, 1.5943112491, -0.6687456829, 0.8647544501\Version=ES64L-G09RevE.01\St
ate=1-A\HF=-575.288294\S2=0.731831\S2-1=0.\S2A=0.05181\RMSD=7.857e-09\
RMSF=1.575e-06\Dipole=0.2562299, -0.3587341, 1.0560268\Quadrupole=4.4211
227, -0.5515165, -3.8696062, -1.6289216, -1.0891216, -1.3252727\PG=C01 [X(C
9H12O3)]\@

int-1w

1\1\GINC-R211\FOpt\UM11\6-31+G(d,p)\C9H14O4\ROOT\28-Jun-2016\0\#\ um11/
/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=norama
n # guess=read geom=allcheck\Cumene + H2O + O3 complex\0, 1\C, 1.45721
77487, 1.397804425, -0.6803252397\H, 2.066394234, 2.1045774332, -0.09672605
68\C, 1.4972916009, 0.0055145749, -0.0273833359\H, 1.8564782749, 1.37250742
51, -1.7038533516\O, -1.1833192853, -2.0114815417, -0.2717634819\O, -1.7475
597516, -0.8978600147, -0.4097995087\O, -1.4478112499, -0.250688582, -1.448
9931364\H, 0.9213250431, -0.6830615985, -0.6687253262\H, 0.4245231144, 1.77
5234764, -0.7058112814\C, 0.8322956272, 0.0559059872, 1.3509947164\H, 1.336
6853646, 0.78493289, 2.0029203971\H, -0.210356533, 0.3924827402, 1.25741840
57\H, 0.853992614, -0.9238720248, 1.8494584088\H, -2.2864153946, 1.86298472
48, -0.5566433488\O, -2.0475891592, 1.8269077306, 0.376519883\H, -2.3646539
289, 2.6372750638, 0.7873155864\C, 2.9241006478, -0.5223317021, -0.00906771
51\C, 3.4550101801, -1.0887857735, -1.1737725554\C, 3.751521696, -0.4226098
078, 1.1116164848\C, 4.7700551684, -1.5408380349, -1.2222588675\H, 2.816079
9077, -1.1774539915, -2.057036446\C, 5.0710924975, -0.8743110755, 1.0695962
119\H, 3.3647533756, 0.0074024679, 2.0368538905\C, 5.5861802641, -1.4340324
457, -0.0961763382\H, 5.1592924125, -1.9828363448, -2.1410384772\H, 5.69893
4621, -0.7895267181, 1.9582988589\H, 6.6170336501, -1.7895905111, -0.127583
3367\Version=ES64L-G09RevE.01\State=1-A\HF=-651.7186465\S2=0.350738\
S2-1=0.\S2A=0.002671\RMSD=9.952e-09\RMSF=8.160e-06\Dipole=-0.8719433, 0.
8101606, -0.1636804\Quadrupole=4.1384294, -1.5272674, -2.611162, -7.887954
6, 2.1421247, 1.7704493\PG=C01 [X(C9H14O4)]\@

TS1aw

1\1\GINC-R218\FTS\UM11\6-31+G(d,p)\C9H14O4\ROOT\01-Jul-2016\0\#\ um11/
6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts, calcfc, noeigen, maxcyc
=200) freq=noraman # guess=read geom=allcheck\TS for O3--H2O H-abstra
ction on Cumene\0, 1\C, 0.7052476686, -0.7440770082, 1.5408679311\C, -0.09
28551307, 0.5421812846, 1.3800237107\H, 0.9835943058, -0.8902647545, 2.5967
15862\H, 0.1440278841, -1.6262147459, 1.2065954156\O, -0.15284685, 0.719117
1597, -1.2045937486\O, -0.1005707488, 2.0305127529, -1.3669550175\H, -0.339
8651983, 0.5536067242, 0.1972477517\C, 0.7663204661, 1.786987274, 1.5653499
995\H, 1.1135644244, 1.8327294773, 2.609657494\H, 1.6514185313, 1.735231048
, 0.9151449845\H, 0.2314793438, 2.721654518, 1.3518142014\C, -1.4366561983,

0.5826557756,2.0491069301\C,-1.9507505572,-0.5288897485,2.7308469684\C
, -2.2152098822,1.7500697163,1.993200059\C,-3.1971008568,-0.4739869809,
3.3503804116\H,-1.3684656741,-1.4482876816,2.7945831586\C,-3.460213866
6,1.8019335279,2.6090398639\H,-1.8493427658,2.6314720004,1.4621930813\C,
-3.9573849917,0.6912028048,3.2910103959\H,-3.573846016,-1.3483471186
,3.8831962862\H,-4.0480571928,2.7191152087,2.5524413511\H,-4.935069402
2,0.7342503721,3.773154672\H,1.6294282882,-0.6848617507,0.9517184361\O
, -1.2430296323,2.5911475881,-1.2820365175\O,-0.9715279395,4.6560476727
,0.6193049157\H,-0.9158415627,5.6157813651,0.6484454459\H,-1.082162246
2,4.3915769684,-0.3041506227\\Version=ES64L-G09RevE.01\State=1-A\HF=-6
51.7017848\S2=0.68001\S2-1=0.\S2A=0.048097\RMSD=9.503e-09\RMSF=4.226e-
06\Dipole=0.2457365,0.2576186,0.4125488\Quadrupole=-0.77234,6.8765127,
-6.1041727,-0.6992553,-1.9697546,-4.9849964\PG=C01 [X(C9H14O4)]\@

Methyl isobutyrate

ester

1\1\GINC-R158\FOpt\RM11\6-31+G(d,p)\C5H10O2\ROOT\11-Jun-2016\0\#\# m11/
6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noraman
\TS for O3 ester group O-CH3 H abstraction of acrylates\0,1\C,0.1325
623241,0.8629829166,1.2951717174\H,0.8581629764,1.3050202962,1.9892859
088\H,-0.8791264384,1.1503902146,1.6076406261\H,0.2366985834,-0.225088
2775,1.2622095967\O,0.3844294845,1.3238505253,-0.037968748\C,0.3094969
408,2.6578284591,-0.2094132324\O,0.0503714653,3.4149223364,0.700304095
3\C,0.5703935368,3.0572148223,-1.6501566781\H,1.5266485734,2.588543756
3,-1.9299874266\C,-0.532302965,2.4755244875,-2.5503477972\H,-1.5107070
514,2.897972582,-2.2795305014\H,-0.3324321361,2.7331158867,-3.59893577
08\H,-0.5851868595,1.3836737116,-2.4610090913\C,0.6675893557,4.5756736
461,-1.7703963691\H,1.4523641074,4.9798356065,-1.1190058309\H,0.887802
7887,4.8590590967,-2.8083015396\H,-0.2807646862,5.0424799137,-1.472558
959\\Version=ES64L-G09RevE.01\State=1-A\HF=-346.850139\RMSD=6.474e-09\
RMSF=9.468e-06\Dipole=0.1094122,-0.6277959,-0.4029664\Quadrupole=0.070
6104,-0.6702701,0.5996597,0.8314638,0.1418983,-4.5531354\PG=C01 [X(C5H
10O2)]\@

TS1b

1\1\GINC-R355\FTS\UM11\6-31+G(d,p)\C5H10O5\ROOT\29-Jun-2016\0\#\# um11/
6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcfc,noeigen,maxcyc
=200) freq=noraman # guess=read geom=allcheck\\TS for O3 H-abstraction
on tertC-H Ester subst.\0,1\C,0.4564656073,-1.207398141,0.3456691569
\C,-0.2734120116,-1.8308263924,1.5176834308\C,1.601825239,-1.991985785
3,-0.2510147981\C,0.6633825587,0.2782761923,0.5059601256\H,0.420658750
8,-1.9411608672,2.3663429211\H,-1.1085186374,-1.1961671729,1.834964316
6\H,-0.6458210403,-2.829059713,1.2551788376\H,1.2988835904,-3.03175779
45,-0.4283205396\H,1.9410117257,-1.5454242383,-1.1929334267\H,2.453459
297,-1.9951702754,0.4475304476\O,1.8274981934,0.7086497336,0.008157822
9\O,-0.1702555088,1.0152485423,0.9911913377\C,1.9790539815,2.136083696
8,-0.0298020785\H,1.8925940066,2.5511083851,0.9814572736\H,2.971783103
7,2.3199101912,-0.4488055475\H,1.1962619408,2.5645906324,-0.6693391493
\H,-0.422007971,-1.172165456,-0.5612376392\O,-1.3133572091,-0.99738737
59,-1.4969149068\O,-1.2489725882,0.324690003,-1.7433361075\O,-0.156099
0285,0.6596878354,-2.2978954769\\Version=ES64L-G09RevE.01\State=1-A\HF
=-572.1619287\S2=0.752958\S2-1=0.\S2A=0.045415\RMSD=7.365e-09\RMSF=2.6
06e-06\Dipole=0.9686969,-0.502127,0.4519661\Quadrupole=-0.8830283,3.64
23147,-2.7592863,2.7498271,0.6621527,-2.5480736\PG=C01 [X(C5H10O5)]\@

int-1

1\1\GINC-R396\FOpt\UM11\6-31+G(d,p)\C5H10O5\ROOT\28-Jun-2016\0\#\# um11/
/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=norama
n # guess=read geom=allcheck\\Ester subst. + O3 complex\0,1\C,0.69294
86654,-1.345788417,-0.0193528168\O,-2.3959827867,-0.5938945392,-1.3975
946677\O,-2.3460299058,0.6234398595,-1.0723762506\O,-1.193278631,1.117
4177793,-0.9461650777\H,0.2685620749,-1.3324050369,-1.0349243946\C,-0.
3720480917,-1.76371993,0.9904203084\H,0.0504900817,-1.7928981452,2.003
6865054\H,-1.2068687092,-1.0499431146,1.0092151403\H,-0.7643837619,-2.
7584687423,0.7405381376\C,1.9075246621,-2.2875678228,-0.0075293057\H,1
.5888440434,-3.3115606521,-0.2438044168\H,2.658081736,-1.976218024,-0.
7445932282\H,2.376064885,-2.2999996686,0.9870785273\C,1.1429061421,0.0

746933319,0.2590927708\O,0.8666870323,0.7245017682,1.2447287124\O,1.9022188778,0.5657745631,-0.7376116377\C,2.3205286933,1.9254680557,-0.5695644527\H,2.9114625075,2.1711488497,-1.4563017128\H,1.4408336561,2.5779814111,-0.4915843975\H,2.9209928285,2.0269764744,0.3429232567\Version=ES64L-G09RevE.01\State=1-A\HF=-572.1890759\S2=0.392182\S2-1=0.\S2A=0.003464\RMSD=9.783e-09\RMSF=4.741e-06\Dipole=0.0877551,-0.0829145,-0.6551074\Quadrupole=2.0397696,1.9038385,-3.9436081,0.7149168,0.0421196,-3.095547\PG=C01 [X(C5H10O5)]\@

TS1a

1\1\GINC-R355\FTS\UM11\6-31+G(d,p)\C5H10O5\ROOT\29-Jun-2016\0\#\ um11/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcfc,noeigen,maxcyc=200) freq=noraman # guess=read geom=allcheck\TS for O3 H-abstraction on tertC-H Ester subst.\0,1\C,0.4564656073,-1.207398141,0.3456691569\C,-0.2734120116,-1.8308263924,1.5176834308\C,1.601825239,-1.9919857853,-0.2510147981\C,0.6633825587,0.2782761923,0.5059601256\H,0.4206587508,-1.9411608672,2.3663429211\H,-1.1085186374,-1.1961671729,1.8349643166\H,-0.6458210403,-2.829059713,1.2551788376\H,1.2988835904,-3.0317577945,-0.4283205396\H,1.9410117257,-1.5454242383,-1.1929334267\H,2.453459297,-1.9951702754,0.4475304476\O,1.8274981934,0.7086497336,0.0081578229\O,-0.1702555088,1.0152485423,0.9911913377\C,1.9790539815,2.1360836968,-0.0298020785\H,1.8925940066,2.5511083851,0.9814572736\H,2.9717831037,2.3199101912,-0.4488055475\H,1.1962619408,2.5645906324,-0.6693391493\H,-0.422007971,-1.172165456,-0.5612376392\O,-1.3133572091,-0.9973873759,-1.4969149068\O,-1.2489725882,0.324690003,-1.7433361075\O,-0.1560990285,0.6596878354,-2.2978954769\Version=ES64L-G09RevE.01\State=1-A\HF=-572.1619287\S2=0.752958\S2-1=0.\S2A=0.045415\RMSD=7.365e-09\RMSF=2.606e-06\Dipole=0.9686969,-0.502127,0.4519661\Quadrupole=-0.8830283,3.6423147,-2.7592863,2.7498271,0.6621527,-2.5480736\PG=C01 [X(C5H10O5)]\@

int-1w

1\1\GINC-R131\FOpt\UM11\6-31+G(d,p)\C5H12O6\ROOT\29-Jun-2016\0\#\ um11/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(maxcyc=200) freq=noraman # guess=read geom=allcheck\Ester subst. + H2O + O3 complex\0,1\C,1.7607243552,-0.0745886555,0.165800487\O,-1.1069554847,-0.5948852903,-0.7820877774\O,-2.0060852975,-0.0647998804,-1.481696451\O,-1.6422588656,0.8811505817,-2.2235993165\H,1.4296533082,-1.0219428279,-0.2848768772\C,1.0597896952,0.1564771988,1.5020976514\H,1.3771064619,1.1146533966,1.9367784595\H,-0.0322578223,0.1851231304,1.391597368\H,1.3222106343,-0.6460477029,2.2043311633\C,3.2917703746,-0.1146380753,0.3163577207\H,3.5744016346,-0.9213206524,1.0054501438\H,3.78450217,-0.2901021844,-0.6481010594\H,3.6624673554,0.8320684549,0.7351366461\H,-2.2141386896,2.6851750335,0.743937547\O,-1.7270062205,1.883383251,0.5345553981\H,-0.823305114,2.1474638542,0.2893067174\C,1.3971775658,1.0117929901,-0.8252754848\O,0.8578662642,2.0707882349,-0.5529572285\O,1.7782720282,0.7143011271,-2.0713478616\C,1.5308303048,1.7273521645,-3.0580171011\H,1.8746672807,1.3081888794,-4.0074918774\H,0.4603377979,1.9591828163,-3.0922961577\H,2.0912302632,2.6362241557,-2.8056021096\Version=ES64L-G09RevE.01\State=1-A\HF=-648.6111833\S2=0.360127\S2-1=0.\S2A=0.002783\RMSD=5.308e-09\RMSF=6.587e-06\Dipole=0.5450801,0.0676248,-0.4555668\Quadrupole=-0.7224505,0.1240934,0.5983571,-1.7614983,0.3733235,-0.4835374\PG=C01 [X(C5H12O6)]\@

TS1aw

1\1\GINC-R157\FTS\UM11\6-31+G(d,p)\C5H12O6\ROOT\28-Jun-2016\0\#\ um11/6-31+g(d,p) int=ultrafine scf=maxcyc=200 opt=(ts,calcfc,noeigen,maxcyc=200) freq=noraman # guess=read geom=allcheck\TS for O3--H2O H-abstraction on Ester subst.\0,1\C,1.1930285079,-0.1640373153,-0.1332584817\C,0.7196872919,-0.7854983896,-1.4250879952\C,2.6279658476,0.3272126565,-0.0873711821\C,0.7383865696,-0.9122122919,1.0973341713\H,1.1572554335,-1.7906423249,-1.5317037249\H,-0.3730254358,-0.9064157967,-1.4447143369\H,1.0374011279,-0.1727699302,-2.2777215491\H,2.8279872143,0.9906954249,-0.9379641493\H,2.8436700787,0.8560144925,0.8475510444\H,3.3120255573,-0.5331125649,-0.1640765294\O,1.1493227179,-0.3359858592,2.2267073831\O,0.0499093414,-1.9152248564,1.07860349\C,0.6263738772,-0.9107368544,3.4348755133\H,0.9317563616,-1.9608521611,3.5133466427\H,1.0422612995,-0.315945585,4.2519140742\H,-0.4692249904,-0.848275309,3.4205752332\H,0.5173073256,0.8870228088,-0.0196532672\O,-0.3450978812,1.87192853

04,0.0114082883\O,-1.5315945052,1.2409742603,-0.0475271129\O,-1.811080
0982,0.6316453577,1.0333013488\H,-2.9156544643,-1.2989547391,-0.050838
5079\O,-2.335517436,-1.8630230334,-0.5731171532\H,-1.6141437408,-2.123
8065202,0.0194168007\Version=ES64L-G09RevE.01\State=1-A\HF=-648.57871
65\S2=0.760148\S2-1=0.\S2A=0.044503\RMSD=8.074e-09\RMSF=4.935e-06\Dipo
le=1.4054972,0.4155646,0.8104475\Quadrupole=1.2647754,-5.7484372,4.483
6618,-3.3667874,-4.2746028,-3.5345441\PG=C01 [X(C5H12O6)]\@