Experimental and Theoretical Study of the Kinetics of the OH + Propionaldehyde Reaction Between 277K and 375K at Low Pressure

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Supporting Material

Below are the geometries (in Angstroms), energies (in Hartrees) and vibrational frequencies for several species involved in the OH + propionaldehyde reaction at various levels of theory.

OH

B3LYP/6-311G++(2d,2p)

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                         Standard orientation:
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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          8             0        0.000000    0.000000    0.108250
    2          1             0        0.000000    0.000000   -0.866000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):      0.0000000    561.6017003    561.6017003
 Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) =  -75.7643231693

Frequencies --  3717.3545

Zero-point correction=                           0.008469 (Hartree/Particle)
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MP2/6-311G++(2d,2p)

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                         Standard orientation:
    ---------------------------------------------------------------------
      Center     Atomic     Atomic              Coordinates (Angstroms)
      Number     Number      Type              X           Y           Z
    ---------------------------------------------------------------------
      1          1             0        0.000000    0.000000   -0.858942
      2          8             0        0.000000    0.000000    0.107368
    ---------------------------------------------------------------------
Rotational constants (GHZ):      0.0000000    570.8690760    570.8690760
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UHF) =  -75.4168439640

EUMP2 =    -0.75597371391588D+02

Frequencies --  3824.6265
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Zero-point correction= 0.008713 (Hartree/Particle)

UMP4(SDTQ)= -0.75614134760D+02 (single point MP4(SDTQ)/6-311++G(2d,2p))

Propionaldehyde

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.687160	-0.288547	-0.176033
2	1	0	-1.830918	-1.058093	0.583888
3	1	0	-1.569324	-0.785085	-1.139075
4	1	0	-2.595235	0.311164	-0.215927
5	6	0	-0.471668	0.593118	0.143061
6	1	0	-0.301904	1.343635	-0.627595
7	1	0	-0.643028	1.114759	1.091074
8	6	0	0.784413	-0.221757	0.309270
9	1	0	0.715595	-1.039502	1.058409
10	8	0	1.808913	-0.047970	-0.301069

Rotational constants (GHZ): 25.9674660 4.3143347 4.1594049
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(RB+HF-LYP) = -193.213107701

Frequencies --	79.6332	209.2639	328.6096
Frequencies --	508.6945	761.6657	876.0506
Frequencies --	921.9243	1005.0235	1133.5367
Frequencies --	1162.2015	1277.4818	1331.9935
Frequencies --	1414.9181	1426.5511	1474.0148
Frequencies --	1506.8146	1511.4724	1797.7013
Frequencies --	2860.3915	3016.3470	3040.2404
Frequencies --	3088.7173	3107.5769	3110.1598

Zero-point correction= 0.084181 (Hartree/Particle)

MP2/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.659123	-0.322105	-0.162057
2	1	0	-1.793546	-1.019198	0.662267
3	1	0	-1.497195	-0.898984	-1.068891
4	1	0	-2.581243	0.239323	-0.277565
5	6	0	-0.479507	0.619842	0.100512
6	1	0	-0.308591	1.293058	-0.734522
7	1	0	-0.683202	1.216208	0.991256
8	6	0	0.776295	-0.166653	0.353010
9	1	0	0.727361	-0.865972	1.208850
10	8	0	1.788803	-0.093868	-0.316273

Rotational constants (GHZ): 24.8308680 4.3941767 4.2411481
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(RHF) = -192.012434569

EUMP2=   -0.19269121182268D+03

Frequencies --	76.2987	224.7683	330.6526
Frequencies --	510.9753	781.2752	887.8479
Frequencies --	930.3803	1030.3695	1142.2449
Frequencies --	1176.0065	1291.9741	1346.2360
Frequencies --	1428.2776	1437.9173	1493.0426
Frequencies --	1528.9872	1532.6886	1747.6090
Frequencies --	2931.1766	3080.8866	3084.1045
Frequencies --	3154.3712	3172.0184	3177.4242

Zero-point correction=   0.085426 (Hartree/Particle)

UMP4(SDTQ)= -0.19275414863D+03 (single point MP4(SDTQ)/6-311++G(2d,2p))

OH-Propionaldehyde pre-reactive Complex (alpha)

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.493800	0.639542	-0.184580
2	1	0	3.530472	0.307634	-0.200831
3	1	0	2.254832	1.046841	-1.166511
4	1	0	2.414197	1.446285	0.545057
5	6	0	1.564598	-0.531857	0.169316
6	1	0	1.618816	-1.330896	-0.568215
7	1	0	1.859924	-0.945139	1.140005
8	6	0	0.137094	-0.089849	0.300726
9	1	0	-0.042228	0.740572	1.011560
10	8	0	-0.790197	-0.570013	-0.310998
11	8	0	-3.486724	0.396449	0.019401
12	1	0	-2.593601	0.016197	-0.141057

Rotational constants (GHZ):   16.6301141   1.4362035   1.3781503
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) = -268.986746445

Frequencies --	33.9568	43.2756	75.5456
Frequencies --	160.1333	216.2130	331.1916
Frequencies --	464.6998	523.9681	571.0203
Frequencies --	766.9462	880.5336	929.1898
Frequencies --	1005.2479	1137.1141	1168.7476
Frequencies --	1277.1545	1332.9408	1416.5893
Frequencies --	1431.1793	1473.4158	1507.3586
Frequencies --	1511.6069	1780.6725	2902.3007
Frequencies --	3018.1527	3043.8719	3094.0615
Frequencies --	3112.6743	3115.5473	3534.5076

Zero-point correction=   0.095364 (Hartree/Particle)

MP2/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.334921	0.710286	-0.241683
2	1	0	3.398548	0.524649	-0.130105
3	1	0	2.123811	0.852765	-1.298082
4	1	0	2.099880	1.635679	0.279104
5	6	0	1.523534	-0.462384	0.321965
6	1	0	1.721785	-1.385073	-0.215238
7	1	0	1.779262	-0.607954	1.372420
8	6	0	0.058328	-0.162697	0.248253
9	1	0	-0.280885	0.730814	0.799331
10	8	0	-0.749330	-0.821126	-0.388718
11	8	0	-3.233637	0.541615	0.064182
12	1	0	-2.479355	-0.026025	-0.182351

Rotational constants (GHZ): 12.4916602 1.6233232 1.5191861
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UHF) = -267.437215775

EUMP2= -0.26829874920166D+03

Frequencies --	40.0344	55.0621	75.0568
Frequencies --	174.2389	229.7165	336.2499
Frequencies --	476.5538	518.5319	608.5691
Frequencies --	788.3203	895.8769	939.8188
Frequencies --	1030.2407	1147.0935	1183.5750
Frequencies --	1293.0228	1347.8995	1431.4361
Frequencies --	1444.7962	1493.2846	1529.3002
Frequencies --	1533.1124	1736.5384	2973.9489
Frequencies --	3084.2957	3087.1738	3158.3537
Frequencies --	3175.8800	3181.4173	3643.4903

Zero-point correction= 0.097079 (Hartree/Particle)

UMP4(SDTQ)= -0.26837842170D+03 (single point MP4(SDTQ)/6-311++G(2d,2p))

OH-Propionaldehyde Transition State (alpha)

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.050021	-0.838253	-0.290469
2	1	0	-1.582003	-1.789769	-0.036651
3	1	0	-2.006082	-0.718108	-1.372495
4	1	0	-3.097753	-0.893823	0.000267
5	6	0	-1.361399	0.333024	0.424374
6	1	0	-1.802392	1.291815	0.155488
7	1	0	-1.458486	0.204798	1.507570
8	6	0	0.111641	0.382478	0.125114
9	1	0	0.670834	-0.564723	0.339658
10	8	0	0.707772	1.331158	-0.318155
11	8	0	2.609044	-0.929981	0.077599
12	1	0	2.540027	-0.003093	-0.223506

Rotational constants (GHZ): 7.2656538 2.2236260 1.8179578
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) = -268.983616583

Frequencies --	-116.7681	47.2987	82.7749
Frequencies --	146.5394	210.3568	325.3796
Frequencies --	381.6909	492.4664	554.1926
Frequencies --	766.6967	879.3119	925.0257
Frequencies --	1003.9254	1130.0092	1160.1699
Frequencies --	1275.5713	1325.4053	1402.1499
Frequencies --	1424.5639	1472.1549	1507.2955
Frequencies --	1510.9081	1789.5788	2712.7187
Frequencies --	3022.2097	3045.3362	3093.2524
Frequencies --	3112.5741	3114.6173	3655.5090

Zero-point correction= 0.094703 (Hartree/Particle)

MP2/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.575129	-1.044842	-0.364662
2	1	0	-0.799917	-1.806461	-0.372198
3	1	0	-1.741663	-0.717454	-1.387404
4	1	0	-2.492716	-1.494528	0.001651
5	6	0	-1.167127	0.134060	0.523695
6	1	0	-1.897562	0.938447	0.505641
7	1	0	-1.040856	-0.206601	1.551383
8	6	0	0.160649	0.683084	0.075514
9	1	0	0.990798	-0.136845	0.089761
10	8	0	0.407531	1.802632	-0.285760
11	8	0	2.060574	-1.139441	0.090230
12	1	0	2.726720	-0.515901	-0.231874

Rotational constants (GHZ): 4.6090428 3.3380025 2.1171927
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UHF) = -267.407328423

EUMP2=   -0.26828407745941D+03

Frequencies --	-1056.7312	52.1938	65.0819
Frequencies --	83.1920	173.2097	227.0727
Frequencies --	355.9027	481.6983	694.4497
Frequencies --	792.6750	876.2555	920.1033
Frequencies --	962.6205	1044.8686	1136.7552
Frequencies --	1183.2565	1292.6786	1345.2176
Frequencies --	1432.1899	1454.0387	1487.5543
Frequencies --	1530.5483	1533.2105	1881.9653
Frequencies --	3088.9348	3091.1692	3158.2416
Frequencies --	3179.2523	3182.7935	3804.8486

Zero-point correction=   0.092293 (Hartree/Particle)

UMP4(SDTQ)= -0.26836616063D+03 (single point MP4(SDTQ)/6-311++G(2d,2p))

OH-Propionaldehyde Transition State (beta)

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.381531	1.622780	-0.134851
2	1	0	0.541725	1.523166	-1.206671
3	1	0	1.317460	1.968603	0.305007
4	1	0	-0.376380	2.386529	0.033614
5	6	0	-0.042587	0.300907	0.477527
6	1	0	-0.237815	0.373924	1.552555
7	1	0	-1.020555	-0.052136	0.038476
8	6	0	0.895718	-0.856946	0.255342
9	1	0	0.580526	-1.812142	0.717653
10	8	0	1.921180	-0.786101	-0.373011
11	8	0	-2.568181	-0.546187	-0.309788
12	1	0	-3.036927	-0.130084	0.433649

Rotational constants (GHZ):   6.0533506   2.5154236   1.9420068
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) = -268.980474111

Frequencies --	-37.4551	57.4430	76.2808
Frequencies --	95.6764	153.9650	242.2653
Frequencies --	254.9785	537.7042	665.8034
Frequencies --	726.1468	846.3397	909.7468
Frequencies --	1008.2309	1109.2439	1146.1886
Frequencies --	1232.3898	1342.2068	1374.9539
Frequencies --	1408.6456	1425.6560	1492.7849
Frequencies --	1497.5926	1788.9585	2408.6067
Frequencies --	2905.1305	3032.3299	3048.5909
Frequencies --	3105.0680	3122.6565	3734.6456

Zero-point correction=   0.092836 (Hartree/Particle)

MP2/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.295792	1.620808	-0.143291
2	1	0	0.430208	1.480721	-1.210950
3	1	0	1.242040	1.971916	0.262745
4	1	0	-0.457324	2.385165	0.020514
5	6	0	-0.100525	0.321536	0.516423
6	1	0	-0.317888	0.403538	1.580908
7	1	0	-1.110045	-0.065345	0.040654
8	6	0	0.831666	-0.835378	0.278567
9	1	0	0.526617	-1.788476	0.744190
10	8	0	1.841245	-0.756774	-0.378509
11	8	0	-2.301019	-0.574636	-0.347445
12	1	0	-2.797014	-0.378030	0.459372

Rotational constants (GHZ): 6.0091046 2.9191320 2.1913739
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UHF) = -267.396971713

EUMP2= -0.26827927634185D+03

Frequencies -- -1523.8908 71.8248 95.8744
Frequencies -- 99.2372 165.6877 244.9082
Frequencies -- 260.3716 554.6083 679.8143
Frequencies -- 776.5837 883.3844 920.6707
Frequencies -- 948.3723 1029.4618 1136.0517
Frequencies -- 1175.0171 1223.8776 1371.2974
Frequencies -- 1411.2251 1426.1814 1444.4597
Frequencies -- 1513.1360 1516.0759 2123.6073
Frequencies -- 2969.1332 3091.3424 3120.4584
Frequencies -- 3172.1006 3193.4315 3808.9067

Zero-point correction= 0.092100 (Hartree/Particle)

UMP4(SDTQ)= -0.26836023093D+03 (single point MP4(SDTQ)/6-311++G(2d,2p))

OH-Propionaldehyde Transition State (gamma)

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.788209	1.086617	-0.359028
2	1	0	0.639270	1.075134	-1.442372
3	1	0	1.547944	0.205318	-0.114655
4	1	0	1.314065	1.992788	-0.049248
5	6	0	-0.486221	0.829995	0.437152
6	1	0	-0.247027	0.811518	1.510097
7	1	0	-1.217267	1.630948	0.269840
8	6	0	-1.139275	-0.492990	0.090847
9	1	0	-0.477937	-1.381421	0.162837
10	8	0	-2.300637	-0.610549	-0.243322
11	8	0	2.370226	-0.887154	0.156768
12	1	0	2.907955	-0.894388	-0.657896

Rotational constants (GHZ): 7.7530580 2.2439165 1.8710388
Standard basis: 6-31+G(d,p) (6D, 7F)

E(UB+HF-LYP) = -268.900525006

Frequencies --	-434.6672	47.9654	68.4661
Frequencies --	98.9843	121.9960	327.5370
Frequencies --	368.9405	505.9173	684.7716
Frequencies --	786.0602	891.1578	916.3329
Frequencies --	1034.5610	1121.7301	1136.8002
Frequencies --	1227.5355	1268.0821	1310.0082
Frequencies --	1355.4869	1380.9694	1420.5930
Frequencies --	1454.7799	1478.1103	1803.1685
Frequencies --	2943.2723	3026.2746	3075.6858
Frequencies --	3085.0057	3152.8982	3737.4978

Zero-point correction= 0.090741 (Hartree/Particle)

MP2/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.109187	0.040382	0.048287
2	1	0	2.270475	0.148016	1.119092
3	1	0	2.156316	1.027005	-0.403494
4	1	0	2.920325	-0.560575	-0.351126
5	6	0	0.757974	-0.621679	-0.242513
6	1	0	0.579237	-0.685238	-1.311973
7	1	0	0.717612	-1.619178	0.187811
8	8	0	-0.807085	1.203341	-0.209202
9	6	0	-0.318241	0.224680	0.372746
10	1	0	-0.395906	0.154251	1.466827
11	8	0	-1.867750	-0.695905	0.085899
12	1	0	-2.142897	-0.384066	-0.791827

Rotational constants (GHZ): 10.0787077 3.1458869 2.6294385
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UHF) = -267.401720316

EUMP2=   -0.26827075702927D+03

Frequencies --	-820.1047	101.7791	199.2868
Frequencies --	227.5988	256.7658	333.9294
Frequencies --	483.4892	531.1763	814.2528
Frequencies --	889.8197	908.1878	1019.6675
Frequencies --	1033.1504	1126.2177	1188.0021
Frequencies --	1290.9018	1344.1778	1407.0325
Frequencies --	1429.9420	1497.8689	1527.9865
Frequencies --	1532.1954	1628.7999	3008.3750
Frequencies --	3084.8110	3110.3190	3161.6331
Frequencies --	3178.4297	3186.2718	3753.4458

Zero-point correction=   0.098543 (Hartree/Particle)

UMP4(SDTQ)= -0.26835759425D+03 (single point MP4(SDTQ)/6-311++G(2d,2p))

OH-Propionaldehyde Transition State (OH addition)

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.161883	-0.015341	0.063723
2	1	0	2.325341	0.040643	1.141003
3	1	0	2.281777	0.985695	-0.349266
4	1	0	2.939543	-0.651750	-0.356468
5	6	0	0.772613	-0.586904	-0.264604
6	1	0	0.612671	-0.610259	-1.342010
7	1	0	0.682778	-1.601672	0.123653
8	8	0	-0.799917	1.249250	-0.208541
9	6	0	-0.294256	0.266308	0.366226
10	1	0	-0.390622	0.182103	1.459381
11	8	0	-1.958084	-0.737868	0.097607
12	1	0	-2.228915	-0.420197	-0.780882

Rotational constants (GHZ):   9.5947448   2.9689820   2.4775041
 Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) = -268.975255512

Frequencies --	-361.8305	83.9407	179.2801
Frequencies --	220.8528	231.1290	298.3687
Frequencies --	436.6551	504.6098	787.6043
Frequencies --	802.3875	885.8377	962.8380
Frequencies --	1000.8564	1096.3896	1162.9379
Frequencies --	1276.2913	1329.4959	1378.2646
Frequencies --	1415.7167	1484.2709	1506.3879
Frequencies --	1511.5871	1562.8311	2962.9698
Frequencies --	3040.3544	3056.7540	3091.9546
Frequencies --	3108.4953	3116.2936	3729.1150

Zero-point correction=   0.096194 (Hartree/Particle)

H2O

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.116780
2	1	0	0.000000	0.762889	-0.467119
3	1	0	0.000000	-0.762889	-0.467119

Rotational constants (GHZ): 828.0800258 430.8030663 283.3777152
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(RB+HF-LYP) = -76.4620395085

Frequencies -- 1638.8808 3823.4771 3925.3988

Zero-point correction= 0.021387 (Hartree/Particle)

MP2/6-311G(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.117561
2	1	0	0.000000	0.756279	-0.470243
3	1	0	0.000000	-0.756279	-0.470243

Rotational constants (GHZ): 817.1151949 438.3673434 285.3059332
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(RHF) = -76.0560950835

EUMP2= -0.76296294603139D+02

Frequencies -- 1659.7985 3865.3724 3985.5566

Zero-point correction= 0.021667 (Hartree/Particle)

UMP4(SDTQ)= -0.76309214210D+02

OH + Propionaldehyde Product (alpha)

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.716368	-0.293166	0.062528
2	1	0	1.859627	-0.870341	-0.849820
3	1	0	1.668058	-0.990533	0.898186
4	1	0	2.588078	0.343807	0.206258
5	6	0	0.448958	0.556762	-0.020265
6	1	0	0.286025	1.147726	0.885315
7	1	0	0.511829	1.251294	-0.862797
8	6	0	-0.801154	-0.263606	-0.284530
9	8	0	-1.887331	-0.110237	0.147057

Rotational constants (GHZ): 33.6516741 4.2285986 4.0250983
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) = -192.563049437

Frequencies -- 60.4560 221.7335 336.7810
Frequencies -- 489.6119 746.0762 817.6869
Frequencies -- 1000.0339 1035.6195 1097.1758
Frequencies -- 1265.4114 1316.0565 1423.5437
Frequencies -- 1452.9128 1503.5129 1510.6953
Frequencies -- 1912.3862 3017.9342 3049.1538
Frequencies -- 3062.1240 3111.9370 3116.4107

Zero-point correction= 0.071870 (Hartree/Particle)

MP2/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.657140	-0.349767	0.051793
2	1	0	1.802010	-0.812225	-0.919848
3	1	0	1.507341	-1.138020	0.784093
4	1	0	2.562078	0.189357	0.315366
5	6	0	0.464103	0.604141	0.024859
6	1	0	0.293798	1.072364	0.993847
7	1	0	0.625012	1.384900	-0.715766
8	6	0	-0.801313	-0.125020	-0.393342
9	8	0	-1.838728	-0.184063	0.180306

Rotational constants (GHZ): 29.4802468 4.4059565 4.1817438
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UHF) = -191.394205905

EUMP2= -0.19204550912505D+03

Frequencies -- 28.7741 230.3628 370.3163
Frequencies -- 480.1944 783.6872 843.3136

```
Frequencies --  1022.0942              1067.4643              1116.8660
Frequencies --  1283.4779              1327.8188              1435.2435
Frequencies --  1485.1341              1526.4650              1532.7199
Frequencies --  1896.2596              3082.4970              3093.4422
Frequencies --  3146.4499              3179.8068              3184.6122

Zero-point correction=                           0.073168 (Hartree/Particle)

UMP4(SDTQ)= -0.19210712067D+03 (single point MP4(SDTQ)/6-311++G(2d,2p))
```

OH + Propionaldehyde Product (beta)

B3LYP/6-311G++(2d,2p)

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.505841   -0.409793   -0.000002
    2          1             0        2.160735   -0.335235    0.873931
    3          1             0        2.161024   -0.335044   -0.873694
    4          1             0        1.021529   -1.382826   -0.000153
    5          6             0        0.506286    0.681970   -0.000030
    6          1             0        0.846097    1.711220   -0.000164
    7          8             0       -1.413754   -0.670051   -0.000058
    8          6             0       -0.901575    0.453179    0.000162
    9          1             0       -1.542668    1.350159   -0.000238
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     19.8044203      5.8124535      4.6200581
 Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) =  -192.564880399

Frequencies --   108.7758               269.9734               304.9020
Frequencies --   653.5076               697.8818               884.2381
Frequencies --   943.5054              1014.6799              1070.1865
Frequencies --  1174.6347              1391.7088              1397.8241
Frequencies --  1425.6726              1476.7846              1490.6676
Frequencies --  1568.9318              2948.1800              3009.9756
Frequencies --  3040.4437              3132.8995              3163.4993

Zero-point correction=                           0.071008 (Hartree/Particle)
```

MP2/6-311G++(2d,2p)

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.503814   -0.411699    0.000002
    2          1             0        2.151164   -0.350049    0.874512
    3          1             0        2.151446   -0.349875   -0.874281
    4          1             0        0.992488   -1.367632   -0.000143
    5          6             0        0.518244    0.694547   -0.000036
    6          1             0        0.844559    1.724271   -0.000162
    7          8             0       -1.402176   -0.662034   -0.000063
    8          6             0       -0.917610    0.433542    0.000167
    9          1             0       -1.548936    1.341220   -0.000220
```

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     19.9220340      5.8267142      4.6356347
 Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UHF) =  -191.401203380

EUMP2=       -0.19203105634469D+03

Frequencies --    69.0709               265.7524               268.3943
Frequencies --   593.7263               703.8334               873.1176
Frequencies --   983.4266              1056.0754              1078.0703
Frequencies --  1177.8178              1408.1886              1430.4674
Frequencies --  1455.1770              1505.2813              1510.0705
Frequencies --  1973.3706              2946.0072              3068.2830
Frequencies --  3129.2436              3197.2811              3231.1049

Zero-point correction=                           0.072728 (Hartree/Particle)

UMP4(SDTQ)= -0.19209496097D+03 (single point MP4(SDTQ)/6-311++G(2d,2p))
```

OH + Propionaldehyde Product (gamma)

B3LYP/6-311G++(2d,2p)

```
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        1.656949   -0.396665   -0.053595
    2          1             0        1.756624   -1.151011   -0.819380
    3          1             0        2.261318   -0.491324    0.835935
    4          8             0       -1.688235   -0.248343   -0.258994
    5          6             0       -0.724588    0.017371    0.410347
    6          1             0       -0.711774   -0.195373    1.497018
    7          6             0        0.569749    0.614288   -0.143918
    8          1             0        0.809829    1.498070    0.454225
    9          1             0        0.377226    0.916419   -1.172847
 ---------------------------------------------------------------------
 Rotational constants (GHZ):     24.4158280      4.7419246      4.5903575
 Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) =  -192.541284970

Frequencies --    89.3782               167.0810               324.1053
Frequencies --   497.0036               569.3789               777.8800
Frequencies --   862.7643               994.2781              1065.3521
Frequencies --  1123.6933              1261.9367              1271.4599
Frequencies --  1406.4902              1465.4693              1474.2608
Frequencies --  1787.7499              2895.4636              3023.2040
Frequencies --  3096.1874              3152.8543              3258.2423

Zero-point correction=                           0.069630 (Hartree/Particle)
```

MP2/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.503814	-0.411699	0.000002
2	1	0	2.151164	-0.350049	0.874512
3	1	0	2.151446	-0.349875	-0.874281
4	1	0	0.992488	-1.367632	-0.000143
5	6	0	0.518244	0.694547	-0.000036
6	1	0	0.844559	1.724271	-0.000162
7	8	0	-1.402176	-0.662034	-0.000063
8	6	0	-0.917610	0.433542	0.000167
9	1	0	-1.548936	1.341220	-0.000220

Rotational constants (GHZ): 19.9220340 5.8267142 4.6356347
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UHF) = -191.401203380

EUMP2= -0.19203105634469D+03

Frequencies -- 69.0709 265.7524 268.3943
Frequencies -- 593.7263 703.8334 873.1176
Frequencies -- 983.4266 1056.0754 1078.0703
Frequencies -- 1177.8178 1408.1886 1430.4674
Frequencies -- 1455.1770 1505.2813 1510.0705
Frequencies -- 1973.3706 2946.0072 3068.2830
Frequencies -- 3129.2436 3197.2811 3231.1049

Zero-point correction= 0.072728 (Hartree/Particle)

UMP4(SDTQ)= -0.19209496097D+03 (single point MP4(SDTQ)/6-311++G(2d,2p))

OH + Propionaldehyde Product (OH addition)

B3LYP/6-311G++(2d,2p)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.021387	0.034113	0.122065
2	1	0	2.140925	0.035632	1.206601
3	1	0	2.069469	1.065197	-0.223454
4	1	0	2.868336	-0.505550	-0.302161
5	6	0	0.717196	-0.628908	-0.294535
6	1	0	0.604181	-0.652500	-1.377988
7	1	0	0.650047	-1.654470	0.066296
8	8	0	-0.663094	1.332034	-0.190917
9	6	0	-0.550956	0.096724	0.264728
10	1	0	-0.386330	0.192545	1.363950
11	8	0	-1.668557	-0.746531	0.048881
12	1	0	-2.419181	-0.176459	-0.150507

Rotational constants (GHZ): 9.2074251 3.5549924 2.7937344
Standard basis: 6-311++G(2d,2p) (5D, 7F)

E(UB+HF-LYP) = -269.013627805

Frequencies --	106.1029	194.4821	215.7478
Frequencies --	253.7601	380.6329	422.3064
Frequencies --	572.6666	773.0614	780.9575
Frequencies --	926.1284	1001.4010	1004.8937
Frequencies --	1078.2590	1137.9230	1174.1060
Frequencies --	1228.9357	1276.6993	1287.2449
Frequencies --	1357.7181	1421.6967	1491.9231
Frequencies --	1500.1714	1511.8326	2770.5339
Frequencies --	3041.3316	3064.0472	3092.0226
Frequencies --	3106.1694	3122.0815	3817.9822

Zero-point correction= 0.098218 (Hartree/Particle)