Supplementary Information for:

Mechanism and Kinetics for the Reaction of Methacrolein and Methyl Vinyl Ketone with HO_2 Radical

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The cartesian coordinates and vibrational frequencies of all stationary points at the M06-2X/6-311+G(2df,2pd) level of theory.

MACR+HO_2 reaction:

MACR

COORDINATES

C	1.500621	-0.935076	0.000016
H	1.319445	-2.003023	0.000021
H	2.531669	-0.606939	0.000023
C	0.486646	-0.074676	-0.000002
C	-0.886078	-0.634237	-0.000013
O	-1.880308	0.041518	-0.000003
H	-0.945374	-1.738851	0.000011
C	0.609642	1.414933	-0.000005
H	1.652435	1.723307	-0.000056
H	0.109601	1.833856	-0.873203
H	0.109696	1.833850	0.873251

FREQUENCY

153.6267	187.0489	265.2063
402.8482	433.0467	631.8875
721.7360	845.6866	980.6968
997.2578	1023.8917	1038.5843
1081.1386	1342.2593	1397.8716
1419.0286	1456.7995	1477.0457
1492.2582	1728.1922	1838.0984
2980.2398	3057.0095	3116.8882
3148.1554	3151.2651	3237.5085

OH

COORDINATES

O	0.054961	0.706958	0.000000
O	0.054961	-0.598630	0.000000
H	-0.879377	-0.866625	0.000000

FREQUENCY

1268.3079	1469.5614	3711.5004

Com1

COORDINATES

C	2.800702	-0.388213	-0.180988
H	3.439708	0.457714	-0.402830
H	3.268120	-1.362460	-0.129130
C	1.494016	-0.224296	0.015912
C	0.981741	1.154231	-0.076647
O	-0.176164	1.464186	0.082910
H	1.730356	1.931269	-0.302576

C	0.513745	-1.310428	0.319905
H	1.010434	-2.275174	0.385694
H	0.003720	-1.111200	1.263661
H	-0.258836	-1.355142	-0.449022
O	-2.574598	-0.642570	-0.636047
O	-2.532034	0.141640	0.406386
H	-1.672364	0.621181	0.339121

FREQUENCY

30.2189	52.7139	92.2924
121.3188	185.6619	217.9958
224.0292	294.9315	413.5541
441.4030	618.9168	653.4060
715.0297	849.9127	981.5697
1006.5506	1030.6322	1043.7977
1088.1929	1296.2224	1349.3138
1406.8295	1429.4690	1465.8585
1480.6839	1502.2214	1579.8475
1725.4265	1806.7434	3039.1087
3051.9878	3113.3776	3146.4068
3148.6460	3234.7747	3404.9299

Com2

COORDINATES

C	-2.310146	-0.199816	-0.808808
H	-2.528898	0.575215	-1.532973
H	-2.956523	-1.067180	-0.800276
C	-1.279760	-0.080858	0.025230
C	-0.485548	1.156470	-0.077924
O	0.454185	1.424292	0.637276
H	-0.814677	1.870928	-0.850875
C	-0.876661	-1.084481	1.057091
H	0.090278	-1.518917	0.802208
H	-0.770149	-0.606158	2.030668
H	-1.610030	-1.883954	1.129384
O	1.694407	-0.673991	-0.985949
O	2.406992	-0.310696	0.041630
H	1.858021	0.365339	0.504679

FREQUENCY

37.6195	67.0408	101.1363
119.0783	155.5211	217.9988
223.9584	280.5408	415.9417
432.2917	541.2876	637.5329
713.8479	850.5827	994.8978
1000.7560	1029.8447	1046.7958
1082.7146	1293.8279	1349.4516

1405.7191	1425.0289	1466.3030
1480.4501	1501.3616	1531.2208
1726.0976	1799.3835	3034.0321
3062.6538	3128.0831	3150.1315
3150.5198	3243.7584	3407.4021

Com3

COORDINATES

C	0.181429	1.566863	-0.962352
H	0.075095	1.342856	-2.017699
H	-0.088428	2.563633	-0.636003
C	0.669785	0.656861	-0.119320
C	1.075548	-0.665460	-0.675743
O	1.682914	-1.482340	-0.042667
H	0.797596	-0.839409	-1.731686
C	0.875852	0.851288	1.346335
H	0.576394	1.847297	1.663977
H	0.306176	0.102667	1.898894
H	1.923959	0.688186	1.596680
O	-1.655798	-1.102461	0.213128
O	-2.362492	-0.018228	0.070276
H	-1.723460	0.661686	-0.233583

FREQUENCY

53.6980	81.1316	90.3079
123.1960	139.9135	186.9356
215.8936	268.5340	398.4935
431.1514	457.1746	626.0706
738.2860	841.4138	976.7063
985.3376	1020.5647	1038.3823
1082.8262	1284.4061	1338.1436
1396.5338	1418.3816	1454.8652
1470.0451	1491.9075	1496.4894
1721.4374	1851.8082	2998.7094
3056.8329	3120.5020	3134.2241
3150.4833	3224.2293	3527.7445

Com4

COORDINATES

C	0.183460	0.242320	1.415911
H	0.219051	-0.640406	2.043647
H	0.906826	1.019969	1.620891
C	-0.714777	0.344513	0.435554
C	-1.662422	-0.784845	0.246686
O	-2.506522	-0.800998	-0.607001
H	-1.541678	-1.626586	0.953817
C	-0.864225	1.513734	-0.487393
H	-0.101951	2.266144	-0.298715

H	-0.806094	1.190049	-1.527453
H	-1.850678	1.961001	-0.363486
O	2.889744	-0.244443	0.117586
O	2.153334	-0.419653	-0.943601
H	1.229865	-0.343750	-0.629132

FREQUENCY

31.7410	47.0823	91.4780
121.7003	171.2361	193.0059
205.7588	259.4457	404.5844
417.9346	443.5385	628.7568
720.0770	838.9005	981.8941
1010.8322	1027.3664	1037.0797
1087.3416	1282.0794	1338.7421
1397.6963	1422.3113	1460.8762
1476.7193	1491.5027	1501.0599
1720.7789	1838.7010	2984.2735
3062.7674	3124.8054	3154.0671
3156.5455	3243.4421	3575.1665

TS-HaddO

COORDINATES

C	2.108042	-0.975896	-0.083848
H	1.957414	-1.973139	0.310083
H	3.052272	-0.772429	-0.570617
C	1.169519	-0.043282	0.034965
C	-0.088390	-0.402531	0.725146
O	-0.818011	0.487560	1.260892
H	-0.157596	-1.435990	1.079825
C	1.276948	1.361090	-0.468110
H	0.472977	1.569883	-1.176482
H	1.167501	2.067765	0.353878
H	2.231759	1.525979	-0.961003
O	-1.224677	-0.712006	-0.807796
O	-2.178078	0.083467	-0.548140
H	-1.754916	0.509468	0.475737

FREQUENCY

-780.9345	75.7736	112.1744
175.4842	206.2881	283.8949
389.4293	457.1143	572.0935
623.1460	692.6518	740.8328
758.2350	854.8533	985.0852
989.9623	1045.1306	1056.5361
1069.8109	1121.1089	1341.3108
1366.5069	1396.1666	1418.5868
1454.8995	1481.7957	1492.5192

1637.0691	1744.8069	1919.5853
3054.8140	3092.9581	3115.4555
3155.0820	3156.0837	3242.0962

TS-HaddC1

COORDINATES

C	0.675069	0.965644	1.157156
H	0.586635	0.587928	2.170814
H	1.054196	1.976548	1.066193
C	-0.244031	0.518709	0.211494
C	-1.156382	-0.594537	0.594676
O	-2.168658	-0.848194	0.003798
H	-0.837734	-1.179862	1.476592
C	-0.598809	1.285236	-1.016052
H	0.230661	1.913946	-1.333235
H	-0.886155	0.613311	-1.821476
H	-1.458469	1.922993	-0.799059
O	1.019098	-0.879708	-0.741574
O	2.097173	-0.661505	-0.152710
H	1.674880	0.230070	0.680427

FREQUENCY

-1107.4029	104.9870	142.0448
175.4560	218.0918	250.6917
297.8716	405.8575	452.6413
508.1860	640.6755	664.4125
699.2476	844.4372	977.2822
1017.4940	1023.4111	1052.6995
1066.6596	1285.3074	1351.7751
1383.7645	1412.8436	1439.8341
1447.7141	1475.3992	1484.6200
1588.0369	1619.6965	1850.1422
2994.8687	3056.8158	3122.3407
3125.0777	3156.3786	3210.2517

TS-HaddC2

COORDINATES

C	0.678981	0.170965	1.177184
H	0.756765	-0.717339	1.792884
H	1.140516	1.058858	1.587977
C	-0.338363	0.267225	0.222093
C	-1.328554	-0.829829	0.206339
O	-2.423616	-0.743858	-0.281598
H	-0.989557	-1.773505	0.680353
C	-0.805406	1.611584	-0.298091
H	0.028596	2.308342	-0.371088
H	-1.258335	1.504162	-1.281648
H	-1.561860	2.039130	0.359870

O	2.213293	-0.270471	0.096604
O	1.722781	-0.429556	-1.047352
H	0.544263	-0.188247	-0.754735

FREQUENCY

-1047.1125	109.3836	154.1031
178.9534	194.6913	249.9249
315.9794	386.5367	486.0638
510.9445	679.6565	708.7905
879.2249	891.2522	968.7568
1031.2032	1039.3921	1096.9996
1135.8454	1194.8746	1335.9828
1376.5344	1415.9737	1426.6702
1444.2516	1489.2244	1506.6462
1556.6927	1693.1368	1836.1406
2961.7200	3060.0160	3127.5585
3141.7845	3149.8272	3229.6132

TS-HaddC3

COORDINATES

C	2.307941	-0.857310	-0.427204
H	2.263970	-1.920696	-0.225967
H	3.182242	-0.486703	-0.945074
C	1.332221	-0.044176	-0.040317
C	0.140264	-0.613090	0.680599
O	-0.597173	0.145895	1.398043
H	0.250859	-1.665846	0.995647
C	1.304461	1.432866	-0.267489
H	2.180463	1.760833	-0.821850
H	0.405959	1.716725	-0.819441
H	1.256668	1.958612	0.686067
O	-2.439584	0.300338	-0.213567
O	-1.889274	-0.456056	-0.967477
H	-0.641227	-0.794081	-0.278916

FREQUENCY

-1497.3636	62.8679	82.9020
140.1027	175.6408	191.8528
270.3882	373.0165	421.9364
474.5020	578.0511	598.0634
710.9565	828.8079	896.2322
956.4586	973.1021	1033.7265
1077.2761	1167.3852	1238.5438
1310.3896	1344.1884	1414.4786
1450.8343	1474.1461	1489.9297
1565.6619	1673.0633	1730.4539
2967.8105	3054.4702	3112.4378

3141.6454 3150.3549 3227.7653

P-HaddO

COORDINATES

C	1.946866	-1.158698	0.259765
H	1.609792	-2.044081	0.782683
H	2.979717	-1.135359	-0.060901
C	1.131488	-0.142432	0.021612
C	-0.294613	-0.228441	0.468663
O	-0.676306	0.920147	1.116039
H	-0.501104	-1.131019	1.048476
C	1.518902	1.118941	-0.686761
H	0.871682	1.286238	-1.548964
H	1.398672	1.975552	-0.023953
H	2.551228	1.069420	-1.024385
O	-1.101654	-0.384282	-0.756876
O	-2.360987	-0.336475	-0.469016
H	-1.614272	0.847902	1.326198

FREQUENCY

60.4104	112.5823	149.6261
199.5613	267.4995	355.5056
387.6232	459.0978	544.2721
563.5189	660.4376	733.1491
856.8609	919.8995	975.1271
988.1533	1038.1428	1074.0986
1185.0031	1244.2680	1299.7120
1324.0687	1358.6958	1408.2098
1443.4761	1471.7670	1480.6267
1504.1830	1758.4205	3050.6864
3104.6938	3111.6107	3147.6958
3149.9657	3237.9694	3851.8880

P-HaddC1

COORDINATES

C	-0.017170	0.506024	1.520689
H	0.408433	-0.377852	1.990976
H	-1.049375	0.613231	1.847276
C	0.006585	0.357847	0.013688
C	-0.845696	-0.817307	-0.452506
O	-1.923178	-1.048508	0.009137
H	-0.417770	-1.411466	-1.280161
C	-0.432399	1.612699	-0.722338
H	0.223474	2.440913	-0.458351
H	-0.396730	1.466874	-1.801420
H	-1.452115	1.857491	-0.431791
O	1.365762	0.110364	-0.436663
O	1.790474	-1.053169	-0.052634

H	0.551702	1.385731	1.817552

FREQUENCY

65.0503	163.4617	206.6239
233.5981	252.6664	296.5427
311.8935	354.7296	421.4874
536.1459	632.3139	783.5739
894.7496	944.6610	964.5531
1007.2463	1043.6153	1194.0633
1257.5852	1275.4071	1297.4119
1395.7359	1402.3968	1419.8022
1478.5807	1486.9841	1498.1418
1513.5836	1877.0465	3019.3041
3060.8935	3069.6969	3139.3751
3153.2299	3155.6952	3157.4761

P-HaddC2

COORDINATES

C	0.671561	-0.510444	0.670571
H	0.782799	-1.587435	0.541460
H	0.439183	-0.278768	1.709495
C	-0.357508	0.082928	-0.281875
C	-1.609166	-0.762120	-0.220257
O	-2.698529	-0.334228	0.031304
H	-1.461657	-1.839945	-0.430690
C	-0.631761	1.551692	-0.012244
H	0.290008	2.127817	-0.068074
H	-1.339990	1.948214	-0.736405
H	-1.069122	1.680125	0.977660
O	1.967365	0.083029	0.452989
O	2.464892	-0.268537	-0.689411
H	0.050206	-0.064457	-1.289677

FREQUENCY

72.6871	83.8939	138.3119
245.0466	256.9138	282.1042
359.1542	414.5658	569.7391
687.7556	830.4889	905.1666
952.4478	955.9703	1000.3710
1110.2545	1169.4345	1191.3382
1252.0428	1291.8094	1320.7296
1378.1075	1403.9354	1418.8225
1440.4404	1492.6080	1502.1847
1507.3264	1870.1341	2961.8578
3043.5463	3074.5010	3091.6713
3147.2257	3159.8743	3162.6844

P-HaddC3

COORDINATES

C	-1.462808	-0.998062	-0.162154
H	-1.241628	-2.057927	-0.164877
H	-2.488868	-0.706827	-0.344146
C	-0.515499	-0.097158	0.055622
C	0.899331	-0.539586	0.339762
O	1.860520	0.112162	-0.379756
H	1.013566	-1.628917	0.266782
C	-0.745631	1.382691	0.053580
H	-1.786552	1.619293	-0.154161
H	-0.473614	1.814522	1.019596
H	-0.114328	1.861454	-0.694802
H	1.154907	-0.286206	1.388795

FREQUENCY

70.6732	159.5924	261.3124
392.3386	416.0322	562.6579
710.0206	806.5338	839.7360
962.2056	978.0204	1020.8065
1061.4772	1091.3897	1162.3565
1303.6370	1330.2277	1371.8624
1409.6506	1455.2539	1478.3962
1495.2496	1752.3147	2922.4256
3033.4236	3040.4799	3103.2927
3144.8633	3151.0852	3228.9035

TS-OaddC1

COORDINATES

C	0.508448	-0.582657	1.133746
H	0.429987	-1.649203	1.301985
H	1.227463	-0.050344	1.739647
C	-0.516021	0.081585	0.515001
C	-1.572486	-0.712930	-0.118028
O	-2.484957	-0.227856	-0.742507
H	-1.487225	-1.807353	0.010679
C	-0.552293	1.558909	0.335253
H	0.273646	2.043787	0.849359
H	-0.511881	1.810511	-0.728294
H	-1.498993	1.963568	0.697219
O	1.753436	-0.805494	-0.335023
O	2.292489	0.403252	-0.623760
H	1.873368	0.660378	-1.456097

FREQUENCY

-651.5267	71.3894	112.1226
139.8940	155.9693	221.9037
265.5501	301.9823	417.0506

460.6083	487.9490	638.2273
843.9586	888.4615	973.4523
983.4632	1020.7875	1034.7537
1059.1621	1111.6056	1338.6594
1378.1515	1419.4128	1438.2491
1441.1086	1468.7178	1488.8352
1573.9993	1783.4230	3004.1423
3045.6476	3103.5762	3149.1546
3163.3061	3242.1602	3775.6030

TS-OaddC2

COORDINATES

C	-1.923718	-0.227564	-0.651987
H	-2.082421	0.182040	-1.640315
H	-2.653055	-0.925133	-0.268289
C	-0.767910	0.062283	0.058108
C	0.044904	1.209915	-0.440577
O	0.961509	1.687469	0.175008
H	-0.213621	1.557849	-1.456187
C	-0.646543	-0.293898	1.506446
H	0.397509	-0.339888	1.802648
H	-1.131552	0.475173	2.108239
H	-1.121628	-1.252658	1.702484
O	0.493395	-1.044773	-0.785597
O	1.603813	-1.129275	-0.002453
H	2.094637	-0.309170	-0.176189

FREQUENCY

-691.6343	126.5183	136.1731
191.1319	237.5539	253.6974
300.7230	355.9982	402.0773
425.2552	505.5715	542.3418
626.8736	827.4366	852.1644
970.9917	1006.0836	1012.8920
1038.2293	1070.2454	1324.7087
1355.5008	1412.3907	1441.4306
1470.6747	1478.3626	1499.5070
1527.1320	1824.2062	3008.6985
3066.4961	3137.9022	3172.6008
3174.6509	3279.4174	3710.0411

TS-OaddC3

COORDINATES

C	1.828833	-1.103387	-0.309252
H	1.590399	-2.123342	-0.033907
H	2.735682	-0.942041	-0.876483
C	1.035439	-0.096987	0.031443
C	-0.193563	-0.411973	0.831010

O	-0.786117	0.524627	1.468574
H	-0.189832	-1.419936	1.265689
C	1.298563	1.343383	-0.275682
H	0.480466	1.767418	-0.856179
H	1.362619	1.919154	0.647981
H	2.226887	1.453337	-0.831560
O	-1.451093	-0.709942	-0.232758
O	-1.480564	0.214728	-1.228960
H	-2.279670	0.723890	-1.035511

FREQUENCY

-751.5370	68.6578	145.0198
159.2315	206.4593	277.5128
305.1669	397.9416	429.1538
434.7103	552.8763	647.1829
738.8988	855.8259	967.8509
975.3627	985.9314	1041.8710
1069.9287	1221.1119	1319.9516
1343.2852	1409.4939	1418.2765
1452.8045	1460.0862	1476.6453
1494.8273	1739.5576	3057.5254
3060.7791	3122.0478	3144.8853
3146.0697	3231.7453	3798.7439

P-OaddC1

COORDINATES

C	0.848377	-0.053938	1.010407
H	0.726117	-0.751649	1.842174
H	1.345954	0.848564	1.370449
C	-0.464734	0.266651	0.368200
C	-1.361110	-0.817928	0.080476
O	-2.429139	-0.684003	-0.496736
H	-1.028789	-1.815346	0.416748
C	-0.798682	1.658800	-0.007941
H	-0.798653	2.303961	0.875336
H	-0.030623	2.054764	-0.678262
H	-1.771391	1.710010	-0.489479
O	1.715468	-0.753358	0.129260
O	2.034952	0.141489	-0.927083
H	1.644042	-0.304845	-1.687354

FREQUENCY

34.0953	115.6277	149.3575
175.0723	242.6222	280.7853
295.8334	356.1811	414.3945
530.2613	667.9791	830.5553
931.2454	958.7270	982.1693

1000.3844	1037.0828	1089.9199
1265.0095	1277.6794	1348.5523
1392.1251	1413.7790	1414.2495
1436.7131	1476.5704	1483.1764
1487.3220	1654.3771	2998.3462
3033.4363	3060.6387	3082.9566
3113.4882	3153.9276	3842.8867

P-OaddC2

COORDINATES

C	0.625754	1.591806	-0.772961
H	0.267781	1.803044	-1.768888
H	1.496741	2.100336	-0.392056
C	0.066140	0.447685	-0.013886
C	0.805848	-0.794249	-0.532821
O	1.739253	-1.300017	0.015132
H	0.422743	-1.157371	-1.506296
C	0.203350	0.593600	1.490247
H	-0.244982	-0.261687	1.990023
H	1.258244	0.632832	1.754102
H	-0.290904	1.507101	1.814649
O	-1.290684	0.350446	-0.433210
O	-1.809874	-0.851054	0.133387
H	-2.225732	-1.252311	-0.637470

FREQUENCY

97.3615	158.5612	177.5724
222.6409	231.6693	240.9701
298.5404	313.3889	364.5250
427.5790	518.9196	559.4765
604.9436	789.4291	900.9214
968.8734	982.3988	1003.0901
1044.5353	1165.9902	1237.5640
1271.6368	1390.1264	1406.1922
1414.6395	1443.7534	1489.2868
1497.1303	1865.7949	2967.1217
3070.7046	3153.9261	3163.1442
3175.2998	3294.1012	3868.6997

P-OaddC3

COORDINATES

C	1.924444	-0.935769	-0.450243
H	1.753798	-2.003592	-0.429798
H	2.866940	-0.590711	-0.854865
C	1.018930	-0.070719	-0.020242
C	-0.312075	-0.623318	0.506348
O	-0.702349	0.107129	1.566959
H	-0.157970	-1.665611	0.820790

C	1.209735	1.416219	-0.018604
H	0.476804	1.895890	-0.665463
H	1.075943	1.818483	0.986318
H	2.209896	1.667182	-0.365216
O	-1.312763	-0.741875	-0.486201
O	-1.607032	0.548951	-0.983394
H	-2.294464	0.846241	-0.374232

FREQUENCY

13.8004	144.4455	184.4972
224.7086	263.2945	308.8961
366.3584	399.2584	483.4026
545.7253	702.5949	749.2627
846.1783	948.2119	971.8671
991.0515	1023.3498	1063.9728
1076.4856	1101.7823	1147.1626
1282.5379	1335.3548	1408.8895
1430.1895	1454.2359	1480.2783
1501.4603	1739.7224	3030.9177
3059.6724	3127.3437	3145.0735
3156.6859	3242.4432	3816.7964

TS-absH-CHO

COORDINATES

C	-0.526413	-1.620165	-0.268183
H	0.528750	-1.680166	-0.500136
H	-1.087585	-2.543458	-0.204427
C	-1.115309	-0.445705	-0.063447
C	-0.271226	0.770174	-0.168903
O	-0.624025	1.890472	-0.012962
H	0.944623	0.506938	-0.438581
C	-2.558388	-0.223799	0.272759
H	-2.650555	0.285850	1.231879
H	-3.027654	0.417290	-0.473457
H	-3.091845	-1.170293	0.318568
O	2.164062	0.138623	-0.583567
O	2.499595	-0.407736	0.636062
H	2.895224	0.329935	1.116536

FREQUENCY

-1848.5478	57.2878	76.3998
121.3339	150.7109	160.2788
266.1606	306.9374	413.1549
433.7175	468.7957	550.2850
652.3722	754.6331	864.2477
984.1621	1023.9532	1031.9480
1071.7712	1106.5074	1231.5169

1305.0210	1367.9893	1412.9560
1419.6135	1458.2506	1473.4847
1494.9008	1725.9724	1913.3174
3055.9042	3119.4894	3146.9817
3153.3040	3247.2898	3804.8266

TS-absH-CH_3

COORDINATES

C	-2.447205	-0.613453	-0.368742
H	-3.114499	0.094454	-0.843669
H	-2.771838	-1.643462	-0.312749
C	-1.266330	-0.216340	0.125505
C	-0.910631	1.212814	-0.055404
O	0.173207	1.675827	0.194568
H	-1.715350	1.852966	-0.456599
C	-0.280472	-1.083297	0.754114
H	0.747024	-1.088560	-0.098376
H	0.279047	-0.643640	1.576130
H	-0.575139	-2.115667	0.902629
O	1.689183	-0.782708	-0.745610
O	2.459181	-0.028761	0.100709
H	2.006026	0.830698	0.102468

FREQUENCY

-2015.0120	81.5509	132.9726
165.0620	182.7217	189.7317
292.9199	395.8194	449.0540
536.9565	590.2022	637.1575
655.7650	705.7759	870.6679
965.8048	984.3194	986.7105
1027.2215	1056.0275	1111.7143
1193.0992	1354.6310	1395.4723
1444.4533	1457.2180	1482.6144
1495.2531	1672.2636	1821.9845
3015.5437	3105.3438	3151.0961
3200.3765	3243.4318	3693.8914

TS-absH-CH_2

COORDINATES

C	-0.163149	-1.143732	-0.146447
H	-0.044500	-2.209890	0.001115
H	-1.506868	-0.753669	-0.377651
C	0.717308	-0.166773	-0.120248
C	2.138584	-0.544090	0.168654
O	3.023057	0.263119	0.222238
H	2.325360	-1.619550	0.331538
C	0.444173	1.287389	-0.353012
H	-0.606743	1.460513	-0.563624

H	0.740432	1.861133	0.524651
H	1.054473	1.641807	-1.183342
O	-2.538567	-0.374395	-0.478072
O	-2.691047	0.495140	0.595081
H	-3.131191	-0.048025	1.259660

FREQUENCY

-1546.7493	54.2740	83.0198
100.9911	152.8354	181.7653
231.5935	278.8593	353.7400
412.3194	436.4370	586.3292
660.7750	739.6873	835.6723
920.7146	995.5452	1021.8512
1076.6500	1078.0990	1106.3657
1281.4008	1406.5142	1412.1461
1425.0855	1433.1693	1482.1891
1486.2675	1694.9199	1835.4159
3003.3778	3070.1371	3132.5934
3180.1451	3198.1314	3820.1844

TS-absCH$_3$

COORDINATES

C	-1.954190	-1.649232	-0.178576
H	-3.032291	-1.672815	-0.325261
H	-1.440665	-2.603192	-0.164356
C	-1.323168	-0.503762	-0.027666
C	-1.973283	0.815740	-0.039580
O	-1.415728	1.867142	0.112774
H	-3.069043	0.768958	-0.206394
C	0.639922	-0.439407	0.230101
H	0.496302	-1.127191	1.052291
H	0.716005	-0.826935	-0.775316
H	0.496797	0.621900	0.387836
O	2.336875	-0.409324	0.479019
O	2.896245	0.327270	-0.552628
H	2.958080	1.218535	-0.187794

FREQUENCY

-1152.0275	53.5567	103.0949
132.7081	135.2600	189.8824
221.4653	280.9652	354.7424
380.2722	423.0639	488.1572
593.0719	615.6408	904.3499
982.7431	998.0276	1020.1259
1120.7995	1212.3795	1225.6433
1240.8621	1373.6940	1379.3306
1396.7493	1418.0109	1432.7362

1700.5628	1827.2074	2947.5890
3063.8810	3099.3223	3191.3938
3232.8962	3246.1667	3810.6847

H_2O_2

COORDINATES

H	1.019091	0.632758	0.459120
O	0.700530	-0.115093	-0.057358
O	-0.700456	0.115051	-0.057441
H	-1.019684	-0.632426	0.459271

FREQUENCY

380.1509	1048.6605	1365.8757
1481.2339	3855.2713	3856.5525

P-absH-CHO

COORDINATES

C	-1.490497	-0.949881	0.000034
H	-1.311109	-2.016214	0.000107
H	-2.515691	-0.603341	0.000091
C	-0.471378	-0.098138	-0.000104
C	0.901458	-0.678012	-0.000062
O	1.921998	-0.093853	0.000050
C	-0.571887	1.398140	-0.000013
H	-0.073720	1.810583	0.877387
H	-0.069299	1.811073	-0.874653
H	-1.612348	1.716069	-0.002461

FREQUENCY

140.5094	183.0777	243.4301
399.3337	454.7514	596.1893
757.7825	805.6721	961.8382
1015.1368	1026.1753	1065.8066
1267.6995	1406.1196	1438.7889
1477.8771	1490.1482	1723.8850
1967.0691	3053.4610	3116.1892
3146.6331	3156.9201	3250.6995

P-absH-CH_3

COORDINATES

C	1.578180	-0.820454	-0.000230
H	1.436811	-1.892148	-0.000178
H	2.591887	-0.447365	-0.000426
C	0.499169	0.028697	-0.000060
C	-0.854503	-0.606319	0.000162
O	-1.886836	0.003334	0.000234
H	-0.846882	-1.712612	0.000259
C	0.566792	1.415294	-0.000092
H	-0.342785	1.995958	0.000036

H	1.517835	1.926188	-0.000239

FREQUENCY

150.4856	297.4975	399.2788
456.3057	531.0590	597.5290
609.6481	820.8124	864.6370
896.1264	976.7955	1037.5517
1038.2142	1315.6353	1368.0571
1437.7276	1480.6717	1537.6311
1854.2658	2981.2139	3161.2594
3173.0371	3260.8315	3286.2289

P-absH-CH_2

COORDINATES

C	1.499552	-1.029382	-0.000139
H	1.538724	-2.107510	-0.000133
C	0.547041	-0.127741	-0.000062
C	-0.865626	-0.610891	0.000067
O	-1.807843	0.133179	0.000180
H	-0.996437	-1.707015	0.000104
C	0.748470	1.359129	-0.000071
H	1.805491	1.609208	-0.000309
H	0.268960	1.796627	-0.875175
H	0.269387	1.796572	0.875298

FREQUENCY

149.8786	177.5353	258.7334
366.5676	424.5187	623.5116
751.3409	825.2164	854.7943
991.1970	1044.1890	1072.1551
1240.7193	1406.2700	1417.7899
1477.4895	1481.5741	1685.9237
1830.0819	2999.5099	3061.5059
3124.2769	3165.0212	3244.5091

P-absCH_3-a (CH_2CCHO)

COORDINATES

C	1.810573	0.031720	0.000293
H	2.016774	1.101569	0.000090
H	2.666149	-0.632221	-0.000413
C	0.578637	-0.410573	-0.000239
C	-0.695377	0.312086	-0.000157
O	-1.784948	-0.185456	0.000159
H	-0.566333	1.414899	-0.000336

FREQUENCY

104.2980	255.1123	492.4773
565.1130	878.8542	977.7285

1008.8091	1122.0798	1382.3274
1427.4369	1721.5763	1833.1290
2928.2390	3091.2091	3206.0790

P-absCH_3-b (CH_3OOH)

COORDINATES

C	1.117698	-0.220514	0.021207
H	1.961384	0.467460	0.018623
H	1.159276	-0.863313	-0.858510
H	1.135595	-0.829393	0.927303
O	-0.026420	0.600062	-0.018047
O	-1.146805	-0.267373	-0.102117
H	-1.576648	-0.113178	0.746653

FREQUENCY

196.4808	267.9565	470.5379
958.5349	1119.6229	1187.0421
1228.9856	1412.8314	1462.7468
1479.3561	1518.6976	3051.6266
3127.3064	3147.2225	3845.0343

MVK + HO_2 reaction:

MVK

COORDINATES

C	1.918298	0.168341	-0.000032
H	2.929394	-0.214727	-0.000042
H	1.803757	1.244665	-0.000095
C	0.871296	-0.645370	0.000050
C	-0.545200	-0.188714	0.000022
O	-1.434508	-1.005644	-0.000042
H	0.989968	-1.721965	0.000105
C	-0.834612	1.293135	0.000019
H	-0.398125	1.765866	-0.880049
H	-1.909715	1.441011	0.000131
H	-0.397909	1.765942	0.879936

FREQUENCY

123.9068	155.1597	304.1300
437.7811	493.5704	545.8909
704.2306	781.3688	957.0616
1012.8439	1050.2386	1055.8183
1076.1535	1280.3245	1314.4376
1398.2037	1453.8963	1479.4173
1484.2326	1716.6360	1820.0425
3058.2900	3124.8519	3158.2876
3173.3725	3190.8962	3244.2175

Com1

COORDINATES

C	1.719778	1.796208	-0.000363
H	1.554612	2.864665	-0.000621
H	2.749194	1.461417	-0.000305
C	0.700702	0.945983	-0.000176
C	0.870512	-0.523473	0.000127
O	-0.109272	-1.247032	0.000447
H	-0.330288	1.282279	-0.000290
C	2.249762	-1.122309	0.000105
H	2.167149	-2.204185	0.000299
H	2.803139	-0.794251	-0.879809
H	2.803315	-0.793962	0.879801
O	-2.610628	0.801012	0.000207
O	-2.685845	-0.500885	-0.000304
H	-1.745690	-0.819172	-0.000025

FREQUENCY

55.9091	75.0391	93.6570
148.6986	150.5155	176.5327
227.0628	309.7712	452.9691
511.2730	560.5924	702.2588
738.4427	797.0527	968.1365
1028.4807	1057.1393	1076.6726
1083.0658	1306.2091	1308.5669
1329.2617	1401.4077	1457.0112
1480.3856	1481.4944	1595.9105
1711.4004	1787.9485	3065.3875
3133.6655	3161.4771	3177.3908
3190.6338	3248.6447	3285.1356

Com2

COORDINATES

C	2.933948	0.281832	-0.428840
H	3.897635	-0.020537	-0.814461
H	2.797482	1.335556	-0.223860
C	1.966799	-0.602915	-0.226168
C	0.619292	-0.251471	0.278337
O	-0.210272	-1.136611	0.381225
H	2.103544	-1.655297	-0.440562
C	0.308434	1.172491	0.644280
H	-0.673192	1.229239	1.103211
H	1.062838	1.565469	1.324898
H	0.306650	1.786531	-0.256866
O	-2.395935	0.579020	-0.795191
O	-2.720020	-0.328874	0.084885
H	-1.855984	-0.748863	0.334632

FREQUENCY

38.6602	93.6608	112.6520
140.4793	175.5613	225.2633
245.2993	313.0984	443.0482
501.4091	562.6334	705.8224
724.7231	792.6379	958.6602
1025.8872	1050.7596	1059.6605
1077.2925	1296.1310	1298.5996
1319.6405	1407.8987	1449.7103
1473.8532	1486.0524	1583.9751
1715.5383	1787.9734	3073.0564
3144.3524	3160.0100	3177.3569
3193.0427	3246.6694	3288.0906

Com3

COORDINATES

C	-0.214467	1.695963	0.551977
H	-0.675029	2.656339	0.361046
H	-0.498796	1.190712	1.465263
C	0.653705	1.163771	-0.303114
C	1.330294	-0.153173	-0.101458
O	2.079429	-0.563693	-0.954224
H	0.936783	1.673810	-1.216974
C	1.046803	-0.929003	1.158965
H	1.606598	-1.858332	1.133915
H	1.337845	-0.346244	2.033655
H	-0.020447	-1.139760	1.245546
O	-2.345385	-0.528297	0.365096
O	-2.020871	-0.528132	-0.896330
H	-1.290353	0.119109	-0.977006

FREQUENCY

40.8844	75.6250	92.3227
124.4086	175.8559	188.1432
200.6490	300.9174	404.3988
456.8308	493.7590	542.5363
707.3665	778.7260	956.3674
1035.6990	1055.0103	1059.1725
1077.7070	1273.8899	1283.3711
1310.7280	1402.7352	1453.1193
1478.6942	1485.1786	1488.4538
1707.5603	1826.6555	3061.4194
3129.3813	3159.2701	3174.5987
3177.2311	3248.3303	3561.0351

Com4

COORDINATES

C	-0.079409	1.952910	0.177828
H	-0.550545	2.841663	-0.221549
H	-0.023867	1.868582	1.256497
C	0.440473	1.026776	-0.621892
C	1.170739	-0.190238	-0.149480
O	1.757484	-0.866459	-0.955741
H	0.404156	1.126063	-1.700707
C	1.180926	-0.503839	1.324848
H	1.679964	-1.455424	1.477466
H	1.715206	0.276998	1.868418
H	0.164925	-0.553845	1.715691
O	-1.578001	-1.205548	-0.191665
O	-2.404676	-0.228386	0.052705
H	-1.864677	0.585455	-0.026038

FREQUENCY

47.0826	76.4842	91.3646
131.5113	151.7421	189.1058
204.2967	294.3138	425.2302
466.0304	492.4346	541.8437
718.8776	775.9908	953.6998
1009.6312	1052.6241	1063.4938
1076.8449	1275.5090	1279.5682
1310.2388	1400.8063	1446.9627
1479.9918	1483.3447	1498.6537
1703.3332	1835.2332	3065.7845
3133.3314	3145.6261	3178.8929
3185.8028	3232.9356	3554.0187

Com5

COORDINATES

C	-0.247047	1.726294	0.139323
H	-0.140212	2.802036	0.099677
H	0.645067	1.152070	0.356802
C	-1.423300	1.147067	-0.061910
C	-1.646046	-0.323346	-0.019183
O	-2.759416	-0.764165	-0.183487
H	-2.315446	1.724502	-0.271765
C	-0.464230	-1.230075	0.222009
H	0.279843	-1.093779	-0.563295
H	0.022237	-0.987972	1.167087
H	-0.808042	-2.259639	0.233690
O	2.688551	-0.185228	0.631887
O	2.744660	-0.143487	-0.671733
H	3.609927	-0.513826	-0.916961

FREQUENCY

40.9477	53.0211	71.7687
73.7447	105.8069	130.0671
144.7593	229.9207	307.9540
447.3131	495.4795	547.3970
710.3853	784.1151	960.6358
1027.6781	1053.5305	1057.8749
1078.3007	1268.1264	1283.5988
1317.7643	1401.9530	1454.4210
1463.5057	1482.1519	1485.2929
1717.2305	1819.7919	3066.3087
3134.9045	3159.0530	3176.5042
3189.4484	3246.6267	3677.7844

TS-HaddO

COORDINATES

C	2.363603	-0.638541	-0.222960
H	3.092391	-1.431932	-0.135979
H	2.647025	0.226223	-0.808179
C	1.183736	-0.725271	0.373619
C	0.147808	0.332738	0.335111
O	-0.697616	0.357344	1.292207
H	0.914591	-1.588243	0.970872
C	0.400424	1.592263	-0.441462
H	-0.520613	2.166713	-0.493671
H	1.151062	2.182909	0.086582
H	0.761187	1.380226	-1.445085
O	-1.060429	-0.518514	-0.948183
O	-2.110972	-0.611111	-0.244013
H	-1.666925	-0.124780	0.759523

FREQUENCY

-797.5853	98.7972	125.1862
200.6829	252.8202	277.6953
322.9423	468.7395	507.0642
558.0680	645.4320	709.6715
769.8130	822.4889	984.4525
1008.2391	1049.3207	1058.0070
1067.0203	1092.8069	1310.3929
1324.0870	1398.6906	1413.4942
1456.5177	1473.5409	1488.8502
1625.2019	1732.3479	1910.3934
3059.1258	3136.4570	3166.6362
3170.2752	3205.3377	3257.0206

TS-HaddC1

COORDINATES

C	-0.850865	1.498660	-0.265183

H	-1.457484	2.087318	-0.941485
H	-0.508174	2.016628	0.622771
C	-0.058709	0.492010	-0.799016
C	1.179994	-0.027110	-0.142127
O	2.008116	-0.596584	-0.806609
H	-0.147450	0.200945	-1.837440
C	1.337554	0.186687	1.341236
H	2.167623	-0.414029	1.699095
H	1.545405	1.238940	1.541720
H	0.422700	-0.078094	1.871426
O	-1.154261	-1.146521	-0.142775
O	-2.095487	-0.580632	0.447872
H	-1.737405	0.636706	0.246554

FREQUENCY

-1123.4828	79.7540	121.5065
168.9567	198.9190	304.1016
397.6646	479.1722	500.7872
539.2276	579.4218	679.4869
698.7133	786.3198	953.2570
1014.3223	1035.5721	1062.6597
1077.9219	1265.6761	1271.3182
1301.3326	1400.9548	1428.8103
1448.3311	1475.6287	1483.6128
1574.4188	1632.1970	1835.3470
3062.8184	3130.6766	3134.9430
3171.9450	3195.3646	3222.9840

TS-HaddC2

COORDINATES

C	0.829276	-0.129869	1.229581
H	1.497372	-0.691894	1.866952
H	0.681152	0.901742	1.518716
C	-0.093403	-0.791551	0.421995
C	-1.352736	-0.138599	-0.029242
O	-2.289775	-0.801206	-0.401132
H	-0.153207	-1.872404	0.477445
C	-1.407377	1.373640	-0.026895
H	-2.272168	1.693988	-0.599373
H	-1.506450	1.738310	0.996827
H	-0.497805	1.805413	-0.446292
O	2.223039	0.328608	-0.053701
O	1.775759	-0.134131	-1.131459
H	0.724347	-0.603055	-0.696574

FREQUENCY

-1018.7282	80.2398	117.6411

177.0280	198.9546	310.4640
444.6965	481.2617	500.0629
566.4872	612.3003	685.3809
794.4251	861.4311	922.5157
995.4725	1053.7891	1086.4175
1136.8678	1238.7956	1250.1742
1300.4166	1395.2213	1411.4609
1427.8997	1477.7538	1486.9149
1556.5428	1691.0841	1826.4951
3056.8230	3122.5860	3156.9732
3167.8790	3176.5638	3243.0445

TS-HaddC3

COORDINATES

C	2.471419	-0.867737	-0.295564
H	3.139834	-1.707109	-0.164593
H	2.792524	-0.087858	-0.973360
C	1.322767	-0.801264	0.360995
C	0.339214	0.333351	0.266554
O	-0.461201	0.485887	1.261435
H	1.018734	-1.586476	1.043733
C	0.762196	1.583574	-0.502174
H	-0.074142	2.277418	-0.529004
H	1.596070	2.056697	0.017533
H	1.074071	1.353265	-1.519168
O	-2.496665	-0.349250	0.088811
O	-1.846526	-0.588255	-0.892608
H	-0.485535	-0.180546	-0.515105

FREQUENCY

-1447.3323	61.5619	100.7645
141.6724	160.5558	209.9376
256.1831	298.4580	441.5962
459.7007	535.1940	548.2355
704.6503	798.2947	934.3355
955.8480	985.0892	1047.6026
1057.7356	1089.2323	1226.1330
1239.4774	1299.3745	1388.7505
1440.8085	1481.7834	1489.9332
1562.3498	1674.6373	1711.1496
3061.3428	3137.9081	3151.4223
3156.3667	3170.6213	3237.1195

P-HaddO

COORDINATES

C	2.423631	-0.191909	-0.352038
H	3.318913	-0.796741	-0.382458
H	2.503545	0.821268	-0.722641

C	1.292929	-0.680254	0.124130
C	0.001640	0.073888	0.215631
O	-0.521114	-0.129300	1.472924
H	1.229835	-1.694846	0.498928
C	0.035181	1.532083	-0.185135
H	-0.972343	1.939724	-0.113827
H	0.689355	2.076419	0.491942
H	0.384930	1.648344	-1.208504
O	-0.884907	-0.613130	-0.773844
O	-2.124554	-0.331616	-0.555445
H	-1.429921	0.195359	1.471947

FREQUENCY

104.6615	138.1125	264.4486
277.0797	309.3664	366.6889
393.5911	431.5922	463.9915
497.5373	635.4495	685.1279
797.0703	846.7093	974.1831
1010.8812	1049.4648	1052.1900
1091.9069	1196.3035	1258.3207
1311.8586	1331.5925	1401.5342
1420.3540	1461.5511	1488.8074
1514.4215	1755.6943	3066.8402
3148.0615	3157.0879	3167.5941
3186.1061	3253.5035	3832.8093

P-HaddC1

COORDINATES

C	1.223628	1.491685	-0.086456
H	0.686237	2.427642	0.041266
H	1.321135	1.291110	-1.151144
C	0.443346	0.380766	0.575253
C	-0.988010	0.241835	0.042449
O	-1.553162	1.215661	-0.374187
H	0.371438	0.532308	1.655653
C	-1.638328	-1.111734	0.131584
H	-2.707495	-1.001779	-0.020186
H	-1.222477	-1.765282	-0.635498
H	-1.428611	-1.577634	1.094786
O	1.140889	-0.880764	0.471345
O	1.227754	-1.272038	-0.762404
H	2.212105	1.575453	0.360111

FREQUENCY

46.9365	127.2328	173.8624
189.9536	240.6820	275.4291
335.4973	455.7266	479.3653

575.0704	680.6823	745.7480
896.0387	972.7644	985.2400
1070.4855	1107.7748	1151.0138
1222.0299	1259.9086	1337.7590
1382.6050	1394.4709	1407.8719
1466.7285	1480.6989	1483.7612
1498.2622	1861.6446	3060.3357
3074.5515	3083.4247	3128.4460
3157.9248	3163.7633	3173.2774

P-HaddC2

COORDINATES

C	-1.113398	-0.634746	0.701903
H	-1.853717	-0.494484	1.486789
H	-0.880195	-1.688044	0.570055
C	0.131696	0.184199	0.945017
C	1.256689	-0.163243	-0.018123
O	1.256926	-1.197400	-0.631821
H	0.501488	-0.001240	1.957573
C	2.360254	0.853153	-0.141816
H	3.192676	0.437074	-0.700575
H	1.971220	1.730042	-0.662791
H	2.689159	1.185544	0.843231
O	-1.730514	-0.246279	-0.544592
O	-2.192731	0.961988	-0.487026
H	-0.101526	1.248456	0.891350

FREQUENCY

52.9230	61.7513	131.5684
144.8238	249.9466	331.3691
440.2421	471.2826	540.6973
623.2303	774.6612	820.4224
927.8132	962.9018	1005.6495
1057.2820	1126.6062	1197.5509
1226.3175	1272.5570	1320.9046
1379.2881	1400.6988	1417.2730
1448.3163	1469.2748	1478.3728
1485.9078	1858.2320	3049.6100
3058.1626	3107.2383	3114.2633
3118.8073	3165.4016	3176.2998

P-HaddC3

COORDINATES

C	-1.920545	0.156839	-0.145988
H	-2.915269	-0.253762	-0.249547
H	-1.811096	1.222170	-0.300338
C	-0.892502	-0.618918	0.154132
C	0.536216	-0.155194	0.313398

O	1.400209	-1.012424	-0.323420
H	-1.028354	-1.685861	0.292310
C	0.799631	1.307398	-0.022444
H	1.855569	1.524125	0.120031
H	0.539098	1.504404	-1.061717
H	0.213493	1.967699	0.614858
H	0.808092	-0.320134	1.377182

FREQUENCY

113.4811	241.1315	304.3991
381.7769	417.9776	515.1024
674.3202	805.7015	946.6181
985.4506	999.2555	1027.2888
1044.5244	1106.4658	1182.1481
1197.0416	1254.1702	1323.3142
1398.5063	1455.3687	1492.6284
1504.2172	1732.2778	2901.6060
3065.0887	3144.4374	3154.2980
3158.2768	3169.1139	3245.1816

TS-OaddC1

COORDINATES

C	-0.816875	1.107790	0.747792
H	-1.489799	1.952077	0.792544
H	-0.836554	0.440404	1.597790
C	0.264382	1.137922	-0.089011
C	1.310176	0.101333	-0.111513
O	2.112490	0.082870	-1.022015
H	0.341868	1.884253	-0.869176
C	1.357459	-0.917506	1.002375
H	0.433925	-1.496620	1.025968
H	2.202561	-1.578314	0.837222
H	1.461151	-0.421462	1.968129
O	-2.094586	0.099057	-0.275781
O	-1.698017	-1.192458	-0.373788
H	-1.363095	-1.273320	-1.277673

FREQUENCY

-685.9198	51.0932	97.6687
114.6944	198.0037	263.0674
291.6925	350.8171	479.8139
489.5136	542.7904	549.4838
784.4863	796.7975	934.7032
965.8284	1015.8795	1049.2013
1070.8218	1119.4936	1272.4540
1289.2814	1396.4154	1421.5335
1436.8530	1479.3922	1485.3445

1560.6767	1762.6410	3059.2312
3129.2112	3165.0976	3166.9710
3201.8096	3256.1374	3779.0673

TS-OaddC2

COORDINATES

C	-0.529685	1.970865	0.056312
H	-1.235369	2.698827	-0.314241
H	-0.100267	2.144349	1.032123
C	-0.292617	0.801243	-0.637229
C	0.886723	-0.074788	-0.321409
O	1.175052	-0.963821	-1.084167
H	-0.606219	0.730382	-1.670028
C	1.632011	0.156158	0.963369
H	0.934284	0.106576	1.800343
H	2.397395	-0.605607	1.072933
H	2.090636	1.145413	0.964599
O	-1.635046	-0.335071	-0.041209
O	-1.147324	-1.369535	0.711785
H	-0.800503	-1.993390	0.056755

FREQUENCY

-724.8947	62.2031	95.7347
169.9736	182.5187	262.8579
308.7540	348.3635	469.5541
496.7683	515.0081	539.7937
618.2045	779.7178	872.6813
950.7194	978.6051	1040.7310
1075.4718	1110.6820	1261.2418
1272.2530	1391.5436	1420.2111
1435.5284	1472.2813	1483.6140
1542.6827	1827.9963	3054.0352
3120.8764	3181.0238	3183.4005
3191.7330	3281.9885	3768.6286

TS-OaddC3

COORDINATES

C	2.074996	-1.070759	-0.147241
H	2.573437	-2.020815	-0.014434
H	2.607392	-0.311225	-0.704166
C	0.872525	-0.856878	0.360989
C	0.142532	0.444837	0.269619
O	-0.540168	0.780928	1.305957
H	0.355739	-1.615331	0.934218
C	0.749138	1.547627	-0.563195
H	1.631252	1.927917	-0.048996
H	1.033450	1.194726	-1.551606
H	0.023888	2.352434	-0.651768

O	-1.810030	-1.051856	-0.331897
H	-2.619343	-0.779308	0.121208
O	-1.229922	0.128758	-0.674746

FREQUENCY

-726.7651	90.3276	153.9408
208.5247	226.3792	289.9667
319.7522	366.8652	424.6073
458.7298	486.4887	563.1093
700.9361	775.7041	945.1744
988.3243	1003.7075	1039.3241
1062.8502	1094.4443	1293.1169
1309.0272	1386.5447	1419.3450
1447.5219	1454.8138	1484.6551
1498.4214	1732.6817	3066.3304
3144.1464	3164.3116	3166.2246
3198.3141	3249.2996	3786.7177

P-OaddC1

COORDINATES

C	1.025563	-0.478180	0.881254
H	1.387385	-1.250397	1.563227
H	0.853423	0.438937	1.445470
C	-0.190663	-0.934283	0.156135
C	-1.389404	-0.150995	-0.054990
O	-2.304468	-0.622473	-0.714628
H	-0.173535	-1.907731	-0.318568
C	-1.480952	1.236128	0.537578
H	-0.638170	1.847086	0.213106
H	-2.414841	1.690187	0.221526
H	-1.453898	1.189208	1.627350
O	2.120670	-0.283887	-0.004580
O	1.805780	0.845193	-0.805510
H	1.676515	0.446021	-1.674227

FREQUENCY

58.6082	75.0046	159.2120
185.8749	252.7379	271.6452
359.6339	474.7472	486.4539
500.1104	558.6436	724.2872
816.3983	921.7297	973.4638
1028.2484	1042.2952	1084.1922
1145.1505	1268.9358	1288.4713
1355.5089	1394.6419	1415.9917
1425.1822	1474.5477	1483.0625
1494.3897	1669.6766	3055.5568
3071.1819	3121.5902	3124.1139

3168.0884 3188.6441 3845.7845

P-OaddC2

COORDINATES

C	0.283527	1.749891	-0.421531
H	-0.346785	2.613792	-0.288247
H	0.942600	1.683674	-1.271475
C	0.203921	0.598305	0.515511
C	-0.880248	-0.409117	0.084642
O	-0.604103	-1.561083	-0.125842
H	-0.076551	0.941796	1.517837
C	-2.275023	0.133056	-0.077142
H	-2.349617	0.606748	-1.057800
H	-2.992062	-0.680658	-0.021066
H	-2.495386	0.893345	0.671543
O	1.436228	-0.053128	0.715624
O	1.904054	-0.525804	-0.535158
H	1.435310	-1.371382	-0.596662

FREQUENCY

70.2344	123.7627	141.2237
211.0485	238.2744	274.4457
337.5548	391.5457	430.8200
526.2736	558.1759	583.0783
681.4447	777.9506	927.7473
975.8600	996.1379	1029.8031
1126.4346	1143.9264	1204.0435
1262.6134	1362.9232	1393.4128
1441.3057	1449.0300	1469.2047
1476.9098	1845.0990	3050.6273
3057.2649	3125.5288	3166.6045
3179.1132	3300.4612	3770.3396

P-OaddC3

COORDINATES

C	2.102220	-0.932377	-0.031559
H	2.759303	-1.640760	-0.515956
H	2.447284	-0.468312	0.882789
C	0.917772	-0.650463	-0.541802
C	-0.038408	0.378922	0.053570
O	0.033663	0.269561	1.398809
H	0.537393	-1.121792	-1.439324
C	0.293262	1.809025	-0.378891
H	1.300748	2.049313	-0.052818
H	0.231085	1.869894	-1.463104
H	-0.421231	2.499539	0.064374
O	-1.743019	-1.151441	-0.082902
H	-1.991756	-1.051297	0.845316

O	-1.354633	0.160977	-0.432055

FREQUENCY

63.4599	168.0969	219.7045
240.9843	254.6362	287.9411
329.4685	366.8871	475.0503
501.0988	612.8639	691.3630
790.4529	920.5355	938.0024
999.7296	1006.7289	1023.1024
1060.5859	1136.2560	1175.8223
1200.2165	1317.5195	1386.4419
1431.5785	1437.3532	1478.7808
1492.8780	1716.6686	3075.6105
3153.8463	3163.9296	3175.5493
3190.4988	3244.5919	3807.6483

TS-absH-CH_3

COORDINATES

C	0.357564	1.897116	0.128450
H	0.436603	2.962022	-0.042343
H	-0.602350	1.528617	0.469242
C	1.386834	1.091643	-0.098099
C	1.338813	-0.382558	0.067859
O	2.244975	-1.078893	-0.336800
H	2.333077	1.465426	-0.468792
C	0.159560	-0.999552	0.727637
H	-0.251531	-0.477900	1.587328
H	-0.845902	-0.805916	-0.122622
H	0.235974	-2.075898	0.829259
O	-1.825122	-0.565242	-0.738554
O	-2.612070	0.174036	0.114184
H	-3.224757	-0.475454	0.482202

FREQUENCY

-1942.8165	69.1519	85.7861
104.1901	152.8900	182.4976
309.1516	424.1877	448.5256
461.3834	554.4329	576.1464
637.7528	752.4971	805.0625
959.5716	1013.9412	1029.5991
1052.5464	1065.5937	1092.9602
1154.1161	1294.6344	1319.9743
1419.2044	1438.2771	1451.2444
1467.4333	1710.6125	1770.0843
3114.6102	3161.4847	3211.0415
3217.4544	3248.1228	3816.0113

TS-absH-CH

COORDINATES

C	0.890478	2.000877	0.112838
H	0.313129	2.917162	0.096259
H	1.960049	2.098705	0.290407
C	0.332534	0.827077	-0.068101
C	0.898122	-0.543908	-0.079496
O	0.193148	-1.511883	-0.224956
H	-1.096473	0.728966	-0.312516
C	2.393841	-0.658427	0.099243
H	2.691153	-0.215891	1.049982
H	2.672077	-1.707634	0.074667
H	2.906524	-0.117071	-0.695924
O	-2.126514	0.441669	-0.472506
O	-2.388711	-0.454119	0.556058
H	-1.959687	-1.263288	0.241449

FREQUENCY

-1335.6921	40.8960	92.5573
134.9325	162.2355	184.5716
240.1796	253.9531	389.6625
459.2808	511.2798	538.0362
653.5615	672.4241	775.4943
890.6279	957.1894	987.7374
1048.7324	1077.3531	1145.0384
1281.0629	1386.3357	1417.7528
1443.5890	1473.6025	1473.9900
1479.1395	1728.3099	1799.2247
3064.3531	3101.4310	3137.2330
3177.5035	3206.9931	3756.7226

TS-absH-CH_2

COORDINATES

C	0.245695	1.566142	0.083211
H	0.688132	2.553196	0.041930
H	1.286621	0.658558	0.379092
C	-0.998311	1.191738	-0.089679
C	-1.548054	-0.202660	-0.013366
O	-2.725124	-0.367508	-0.212515
H	-1.756834	1.940539	-0.316298
C	-0.610668	-1.332450	0.304383
H	-0.116649	-1.157607	1.260332
H	-1.173669	-2.259856	0.336078
H	0.174377	-1.392800	-0.450280
O	2.208497	0.065155	0.573923
O	2.426474	-0.643331	-0.598628
H	3.087273	-0.113183	-1.060381

FREQUENCY

-1679.6472	50.3506	74.3991
126.7155	156.9125	206.2615
241.0084	295.5848	422.0881
498.0735	511.2886	514.0930
587.3059	714.9527	776.7546
905.3761	949.7713	1018.2824
1057.0197	1079.4003	1099.0519
1259.7196	1294.8409	1397.0817
1403.2841	1432.2141	1471.2609
1481.4898	1677.2521	1827.5357
3064.5905	3105.6869	3131.0992
3176.9418	3190.7542	3814.1949

TS-absCH$_3$

COORDINATES

C	-1.934310	-1.670919	-0.095873
H	-2.695842	-2.430643	-0.204967
H	-0.914682	-2.008723	0.030341
C	-2.250847	-0.384291	-0.121262
C	-1.249969	0.698070	0.018383
O	-1.473559	1.855104	-0.018108
H	-3.272109	-0.041858	-0.249812
C	0.609981	0.123289	0.278453
H	0.570964	-0.372108	-0.680772
H	0.881932	1.164704	0.331284
H	0.313116	-0.397442	1.178968
O	2.285727	-0.453720	0.530036
O	3.018475	-0.061388	-0.583950
H	3.422349	0.769207	-0.307072

FREQUENCY

-1068.1509	53.0153	104.7061
122.0781	128.0477	208.7885
264.9800	326.8926	362.4026
409.8210	431.8350	489.3844
564.5728	706.5116	898.6635
999.5898	1026.6051	1051.6210
1112.7274	1143.5084	1186.0407
1212.5218	1297.9779	1366.9707
1388.5954	1403.5713	1448.9181
1711.0939	1928.9237	3066.8059
3160.3353	3172.2199	3240.9142
3259.7540	3268.9410	3819.9647

P-absH-CH$_3$

COORDINATES

C	1.928826	0.144027	-0.042195

H	2.913426	-0.301579	-0.013880
H	1.888523	1.218272	-0.163448
C	0.837835	-0.602639	0.056267
C	-0.565857	-0.106116	0.006517
O	-1.485541	-0.917016	-0.043004
H	0.906761	-1.678810	0.159162
C	-0.845451	1.303923	0.025204
H	-0.077502	2.054835	0.118495
H	-1.878999	1.608242	-0.031054

FREQUENCY

54.1175	308.4067	379.9862
436.5840	488.0505	538.6654
701.8931	808.4947	821.1826
990.2090	996.2595	1048.9962
1063.0644	1307.4750	1318.8529
1452.3274	1488.3049	1627.6680
1724.6155	3153.4125	3187.7926
3194.6726	3236.9125	3308.7510

P-absH-CH

COORDINATES

C	-2.176024	-0.163711	0.000001
H	-2.739150	-0.228204	0.926904
H	-2.739163	-0.228193	-0.926894
C	-0.896423	-0.002400	-0.000005
C	0.497446	0.187613	0.000003
O	0.976674	1.320290	0.000000
C	1.378693	-1.041693	0.000002
H	0.803821	-1.964203	0.000104
H	2.019388	-1.010342	-0.880222
H	2.019552	-1.010228	0.880100

FREQUENCY

87.4297	158.5448	180.6255
333.3184	433.6729	549.6880
627.0857	746.5609	912.2424
923.2846	1006.9110	1031.9339
1200.6364	1396.6531	1416.1883
1482.2383	1483.0718	1575.4752
1897.4987	3072.7559	3093.8559
3147.5450	3164.7616	3166.2884

P-absH-CH_2

COORDINATES

C	1.929104	0.258154	-0.000025
H	3.005885	0.231824	0.000012
C	0.939372	-0.593384	0.000016

C	-0.500176	-0.182379	-0.000004
O	-1.363221	-1.023040	-0.000014
H	1.102527	-1.670088	0.000067
C	-0.803285	1.293539	-0.000005
H	-0.356736	1.762241	-0.877284
H	-1.878329	1.442844	-0.000511
H	-0.357675	1.761918	0.877935

FREQUENCY

95.5791	142.7649	271.8151
484.9639	494.3983	541.1128
717.9521	740.8464	856.4942
902.7878	1024.7819	1052.4179
1225.5547	1261.3786	1397.7189
1466.3534	1479.6553	1668.1896
1825.1307	3058.5119	3108.3833
3124.1245	3173.9755	3254.9608

P-absCH_3-a (CH_2CHCO)

COORDINATES

C	-1.727559	-0.191672	0.000307
H	-2.658932	0.357000	0.000569
H	-1.773160	-1.272850	0.000263
C	-0.555340	0.427096	-0.000101
C	0.693712	-0.365062	-0.000345
O	1.802843	0.023226	0.000028
H	-0.455527	1.507868	-0.000225

FREQUENCY

132.9110	315.9831	545.9871
655.2192	885.2994	1012.7288
1042.7954	1103.6197	1288.1932
1427.2682	1694.6706	1973.5917
3151.1906	3165.0838	3252.9013

P-absCH_3-b (CH_3OOH)

COORDINATES

C	1.117685	-0.220576	0.021122
H	1.158938	-0.863385	-0.858583
H	1.135664	-0.829389	0.927242
H	1.961384	0.467361	0.018315
O	-0.026433	0.600115	-0.017860
O	-1.146850	-0.267176	-0.102258
H	-1.575837	-0.114648	0.747243

FREQUENCY

193.2089	267.9171	470.5737
958.5377	1119.5532	1187.0328

1228.9918	1412.8058	1462.7166
1479.3538	1518.6636	3051.7294
3127.4635	3147.3697	3845.4228

Table S1. Topological and Energy Parameters at the Bond Critical Points of the Reactant Complexes in MACR + HO_2 Reaction (All Values in a.u.)

species	interactions	ρ	$\nabla^2\rho_b$	H_b	$-G_b/V_b$
Com1	H8-O4	0.0397	0.1064	-0.0061	0.8426
	O9-H6'	0.0104	0.0348	0.0010	1.1492
Com2	H8-O4	0.0361	0.1124	-0.0029	0.9145
	O9-H6	0.0083	0.0292	0.0009	1.1636
Com3	H8-C1	0.0191	0.0480	0.0004	1.0360
	O9-C2	0.0118	0.0388	0.0011	1.1447
Com4	O9-C1	0.0091	0.0312	0.0010	1.1695
	H8-C2	0.0168	0.0448	0.0009	1.0957

According to the quantum theory of "Atoms in Molecules" (QTAIM),[1-3] the topological analysis based on the electron density function can provide much useful information to analyze the chemical bond, especially for the weak interactions. For the four reactant complexes, we focus on the BCPs of the interactions between the two reactant monomers. Table S1 gives the topological parameters (the electron density ρ_b and the Laplacian of electron density $\nabla^2\rho_b$) and energy parameters (the electron energy density H_b) and the ratio of the kinetic electron energy density G_b and the potential electron energy density V_b ($-G_b/V_b$) at the BCPs in the reactant complexes. The larger value of the electron density ρ_b, the stronger the atomic interaction; the negative Laplacian of electron density $\nabla^2\rho_b$ indicates the atomic interaction is a covalent bond; If $\nabla^2\rho_b$ is positive but H_b is negative, the interaction is partly covalent in nature.[4, 5] Generally, if the values of $-G_b/V_b$ are greater than 1, the interaction is noncovalent; if it is between 0.5 and 1, the interaction is partly covalent in nature; and if it is less than 0.5, the interaction is a shared covalent. In the four complexes, the ρ_b value of H8-O4 bond is rather larger than the other weak bonds, $\nabla^2\rho_b$ is positive and H_b is negative and the value of $-G_b/V_b$ is between 0.5 and 1, indicating that the interaction is partly covalent. For the other weak interactions listed in Table S1, the $\nabla^2\rho_b$ and H_b are all positive,

and -G_b/V_b is larger than 1, indicating these interactions are noncovalent. That is to say, the H8-O4 bond is stronger than the other weak bonds. These results are consistent with the above discussion about the atomic distances of the weak interactions between the two reactant monomers, i.e., the distance of H8-O4 (1.74 Å in Com1 and 1.76 Å in Com2) are shorter than all the other interaction distances (2.23～3.04 Å).

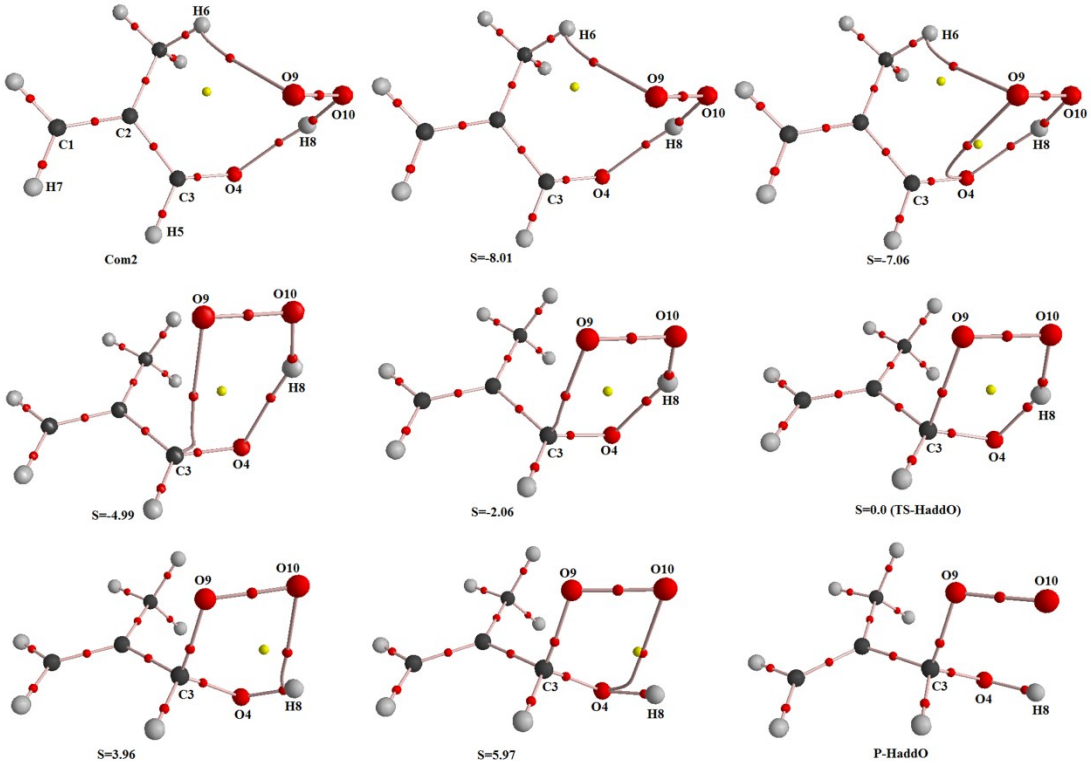

Figure S1. Molecular graphs of the MACR + HO_2 → TSHaddO → PHaddO reaction process.

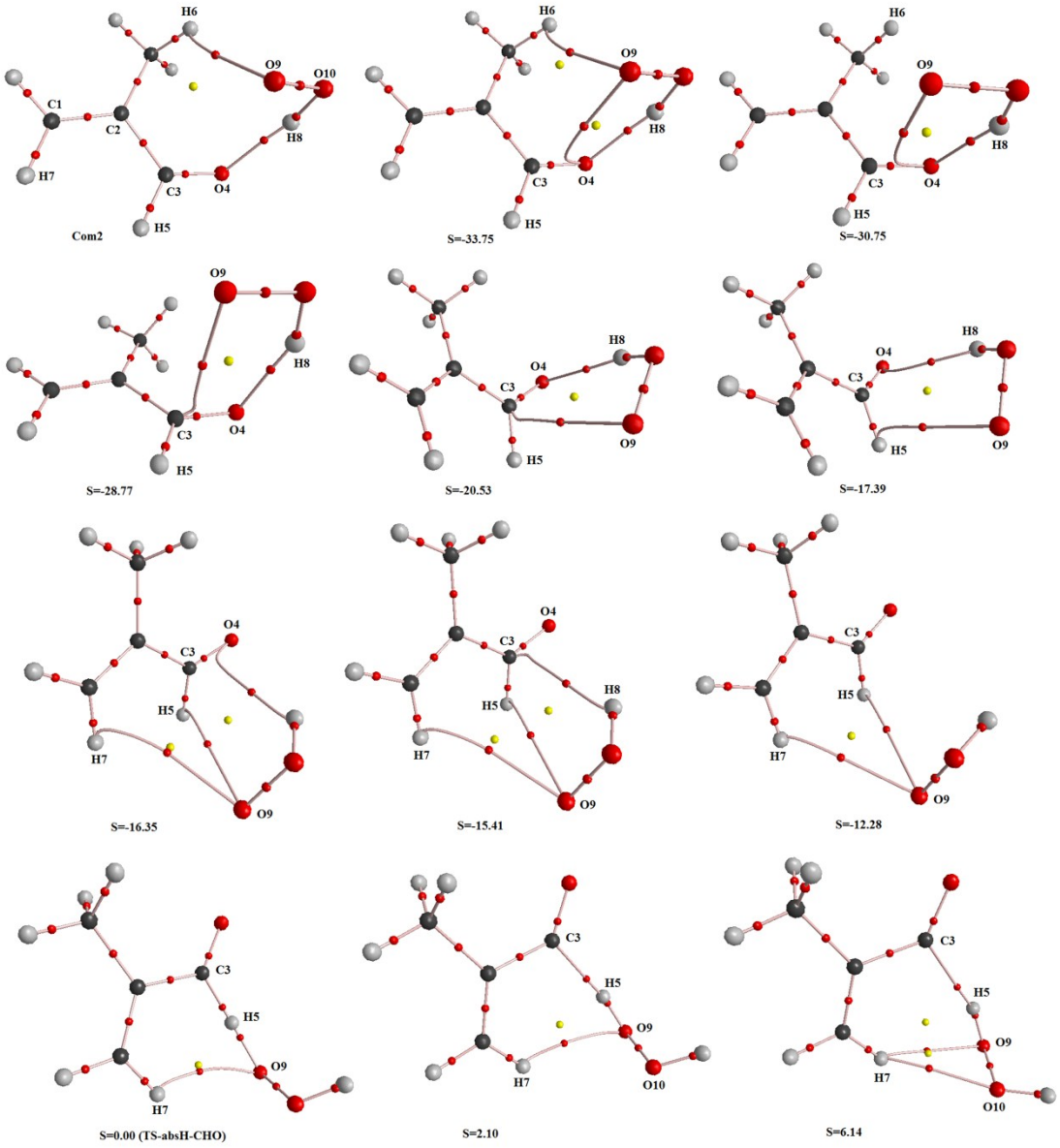

Figure S2. Molecular graphs of the MACR + HO_2 → TSabsH-CHO → PabsH-CHO reaction process.

Table S2. Topological and Energy Parameters at the Bond Critical Points in the MACR + HO_2 → TSHaddO → PHaddO Reaction Process (All Values in a.u.)

	S	H8-O4	H8-O10	O10-O4	O9-H6	O9-O4	O9-C3
ρ	Com2	0.0361	0.3494		0.0083		
	-8.01	0.0366	0.3484		0.0076		
	-7.06	0.0356	0.3491		0.0067	0.0128	
	-4.99	0.0347	0.3488				0.0155
	-2.06	0.0677	0.3199				0.0373
	0.00	0.1649	0.1933				0.0843
	2.06	0.3333	0.0585				0.1827
	3.96	0.3528	0.0309				0.224
	5.97	0.3622		0.0255			0.2299
	PHaddO	0.3662					0.2373
$\nabla^2\rho_b$	Com2	0.1124	-2.6908		0.0292		
	-8.01	0.1132	-2.678		0.0268		
	-7.06	0.1132	-2.6824		0.024	0.0476	
	-4.99	0.1128	-2.6756				0.0541
	-2.06	0.112	-2.3528				0.1164
	0.00	-0.2464	-0.5724				0.1132
		-2.4352	0.1396				-0.238
	3.96	-2.6336	0.1328				-0.4884
	5.97	-2.7156		0.126			-0.5244
	PHaddO	-2.7216					-0.5656
H_b	Com2	-0.0028	-0.734		0.0009		
	-8.01	-0.003	-0.7309		0.0009		
	-7.06	-0.0024	-0.7321		0.0008	0.0012	
	-4.99	-0.0018	-0.7302				0.001
	-2.06	-0.0239	-0.6548				-0.0006
	0.00	-0.1539	-0.2311				-0.0227
	2.06	-0.6849	-0.0138				-0.1512
	3.96	-0.7306	0.0026				-0.2535
	5.97	-0.7524		0.0036			-0.271
	PHaddO	-0.755					-0.2951
$-G_b/V_b$	Com2	0.9172	0.0772		1.1636		
	-8.01	0.9128	0.0775		1.1800		
	-7.06	0.9275	0.0774		1.1818	1.1250	
	-4.99	0.9434	0.0776				1.0877
	-2.06	0.6847	0.0922				0.9802
	0.00	0.3749	0.2758				0.6924
	2.06	0.1000	0.7788				0.3775
	3.96	0.0899	1.0932				0.3414
	5.97	0.0889		1.1481			0.3403
	PHaddO	0.0899					0.3423

Table S3a. Topological Parameters at the Bond Critical Points in the MACR + HO_2 → TSabsH-CHO → PabsH-CHO Reaction Process (All Values in a.u.)

	S	H5-C3	H8-O4	H8-C3	O9-H6	O9-O4	O9-C3	O9-H5	O9-H7	O10-H7
ρ	Com2	0.2881	0.0361		0.0083					
	-35.75	0.2875	0.0351		0.0066	0.0132				
	-30.75	0.2885	0.0346			0.0146				
	-28.77	0.2891	0.0345				0.0155			
	-20.53	0.2896	0.0177				0.0113			
	-17.39	0.2883	0.0097					0.0092		
	-16.35	0.2875	0.0084					0.0088	0.0046	
	-15.41	0.2863		0.0076				0.0087	0.0047	
	-12.28	0.2848						0.0085	0.0056	
	0.00	0.1821						0.1494	0.011	
	2.10	0.0451						0.3512	0.0094	
	6.14	0.0202						0.3625	0.0083	0.0089
$\nabla^2\rho_b$	Com2	-1.1192	0.1124		0.0292					
	-35.75	-1.114	0.1132		0.0260					
	-30.75	-1.12	0.1140		0.0236	0.0484				
	-28.77	-1.1244	0.1124			0.0516	0.0544			
	-20.53	-1.1284	0.0656				0.0428			
	-17.39	-1.1172	0.0336					0.0296		
	-16.35	-1.15	0.0300					0.0280	0.0168	
	-15.41	-1.1456		0.0280				0.0272	0.0164	
	-12.28	-1.089						0.0276	0.0188	
	0.00	-0.448						-0.0624	0.0404	
	2.10	0.0472						-2.5756	0.034	
	6.14	0.0452						-2.7300	0.034	0.0364

Table S3b. Energy Parameters at the Bond Critical Points in the MACR + HO_2 → TSabsH-CHO → PabsH-CHO Reaction Process (All Values in a.u.)

	S	H5-C3	H8-O4	H8-C3	O9-H6	O9-O4	O9-C3	O9-H5	O9-H7	O10-H7
H_b	Com2	-0.3093	-0.0029		0.0009					
	-35.75	-0.3079	-0.0021		0.0007	0.0012				
	-30.75	-0.3099	-0.0016			0.0011				
	-28.77	-0.3109	-0.0017				0.0012			
	-20.53	-0.3118	0.0017				0.0012			
	-17.39	-0.3094	0.0012					0.0007		
	-16.35	-0.3078	0.0012					0.0007	0.0007	
	-15.41	-0.3056		0.0012				0.0007	0.0006	
	-12.28	-0.3027						0.0007	0.0007	
	0.00	-0.145						-0.1013	0.0012	
	2.10	-0.0125						-0.7224	0.0011	
	6.14	-0.0004						-0.7536	0.0012	0.0014
$-G_b/V_b$	Com2	0.0871	0.9145		1.1636					
	-35.75	0.0869	0.9354		1.1591	1.1224				
	-30.75	0.0877	0.9497			1.1028				
	-28.77	0.0872	0.9460				1.1062			
	-20.53	0.0867	1.1308				1.1558			
	-17.39	0.0884	1.1967					1.1186		
	-16.35	0.0896	1.2353					1.1250	1.2593	
	-15.41	0.0902		1.2609				1.1273	1.2143	
	-12.28	0.0926						1.1296	1.2059	
	0.00	0.1854						0.4583	1.1558	
	2.10	0.6603						0.0981	1.1719	
	6.14	0.9672						0.0861	1.1967	1.2188

The topological analysis of electron density on the reaction paths.

The molecular graphs in Figures S1 and S2 depict the forming and breaking of the chemical bonds in the MACR + HO_2 → TS-HaddO → P-HaddO and MACR + HO_2 → TS-absH-CHO → P-absH-CHO reaction processes. The topological and energy parameters at the bond critical points in the two reaction processes are listed in Tables S2, S3a and S3b. From Table S2, it can be seen that for the concerted addition of terminal O and H atoms of HO_2 to the C=O double bond, the values of ρ_b of the forming bonds H8-O4 and O9-C3 increase gradually, while that of the breaking bond H8-O10 decreases gradually. For the forming bond H8-O4, the interaction changes from partly covalent to covalent bond; For the forming bond O9-C3, the interaction character shows from noncovalent to partly covalent, and finally to covalent bond; While for the breaking bond H8-O10, the atomic interaction shows a reverse trends, changing from covalent bond to partly covalent,

and finally to noncovalent; From Table S3a and Table S3b we can see that for the aldehyde-H abstraction processes, the value of ρ_b of the forming bond O9-H5 increases and that of the breaking bond H5-C3 decreases gradually. Before the transition state (S = 0.00), the interaction of H5-C3 shows covalent character while that of the O9-H5 shows noncovalent, and after the transition state, the interaction of H5-C3 shows partly covalent while that of the O9-H5 shows covalent, indicating the breakage of the H5-C3 bond and the formation of the O9-H5 bond.

Table S4. Topological and Energy Parameters at the Bond Critical Points of the Reactant Complexes in MVK + HO_2 Reaction (All Values in a.u.)

species	interactions	ρ	$\nabla^2\rho_b$	H_b	$-G_b/V_b$
Com1	H8-O4	0.0464	0.1024	-0.0106	0.7735
	O9-H5	0.0129	0.0428	0.0011	1.1294
Com2	H8-O4	0.0470	0.1048	-0.0105	0.7780
	O9-H6	0.0084	0.0304	0.0010	1.1786
	O9-C1	0.0091	0.0296	0.0008	1.1404
Com3	H8-C2	0.0164	0.0436	0.0010	1.1111
	O9-H6'	0.0076	0.0248	0.0007	1.1458
Com4	H8-C1	0.0178	0.0456	0.0007	1.0700
	O9-C2	0.0102	0.0344	0.0011	1.1719
	O9-H6'	0.0060	0.0216	0.0008	1.2105
Com5	O9-H7	0.0093	0.0320	0.0009	1.1452
	O10-H6"	0.0062	0.0228	0.0008	1.1951

Table S5. The rate constants of the addition and hydrogen abstraction reaction channels for the reaction of MACR + HO_2 in the temperature range of 200-500 K (The rate constant data to create Figures 6).

	200	250	298	350	400	450	500
TST-add	1.12E-14	7.69E-15	6.22E-15	5.45E-15	5.11E-15	5.00E-15	5.04E-15
TST/Eckart-add	5.69E-14	2.18E-14	1.34E-14	9.87E-15	8.32E-15	7.55E-15	7.20E-15
TST-abs	4.00E-27	1.62E-24	8.47E-23	1.94E-21	1.94E-20	1.22E-19	5.51E-19
TST/Eckart-abs	4.11E-20	1.64E-20	2.34E-20	6.70E-20	2.31E-19	7.81E-19	2.40E-18

Table S6. The rate constants of the addition reaction channel for the reaction of MVK + HO_2 in the temperature range of 200-500 K (The rate constant data to create Figures 7).

	200	250	298	350	400	450	500
TST-add	3.83E-14	1.81E-14	1.15E-14	8.46E-15	7.00E-15	6.21E-15	5.80E-15

TST/Eckart-add	2.13E-13	5.37E-14	2.56E-14	1.56E-14	1.16E-14	9.49E-15	8.37E-15

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