Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Online Supplementary Material

Reactions of a Distonic Peroxyl Radical Anion influenced by SOMO-HOMO Conversion: An Example of Anion-Directed Channel Switching

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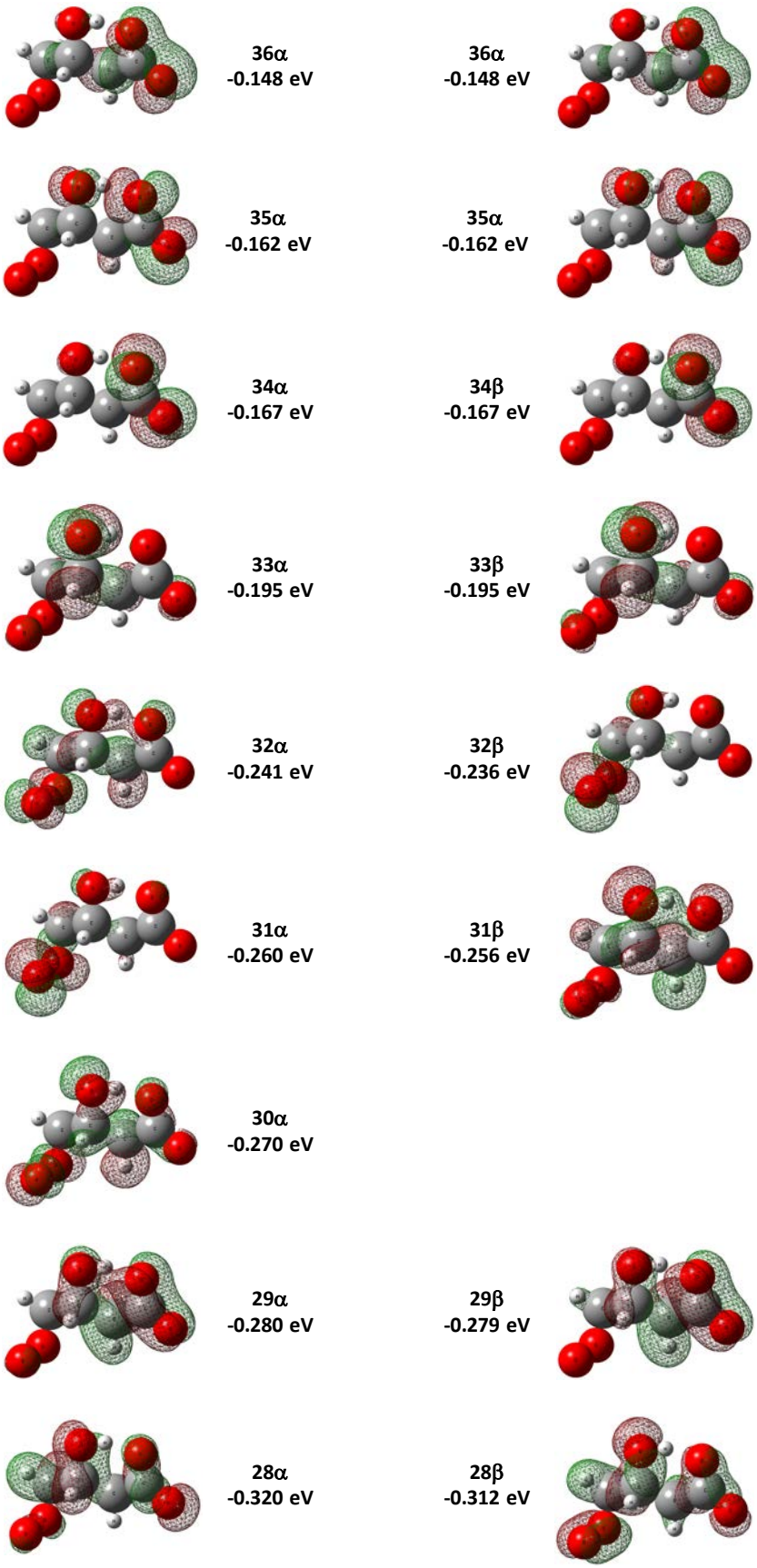
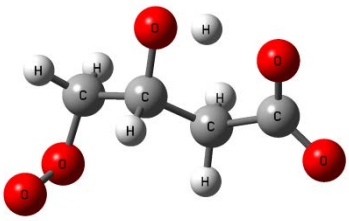
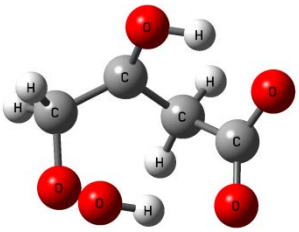


Figure S1: Molecular orbital assignments and energies in the distonic radical anion $^{\bullet}O_2CH_2CH(OH)CH_2C(O)O^-$ (**W1**).



W1



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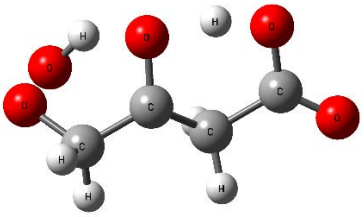

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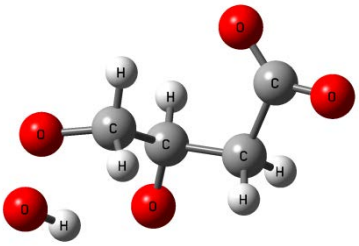
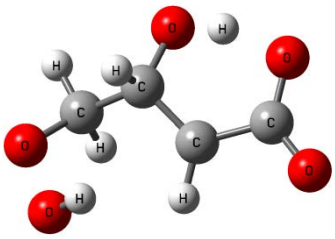
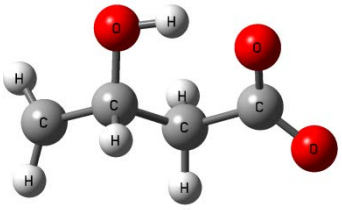


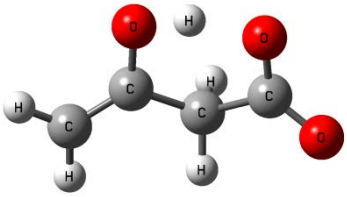
W4



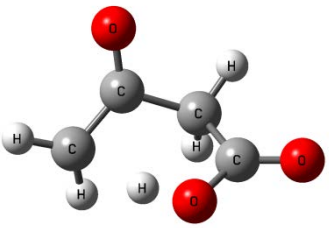
W5



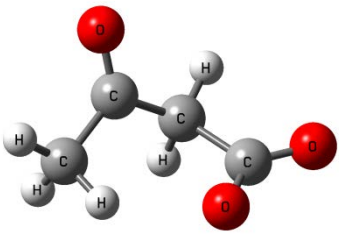
$CH_2CH(OH)CH_2C(O)O^-$



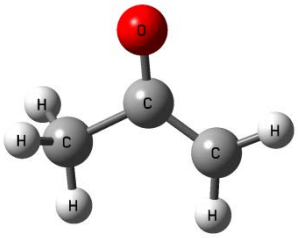
$CH_2C(OH)CH_2C(O)O^-$



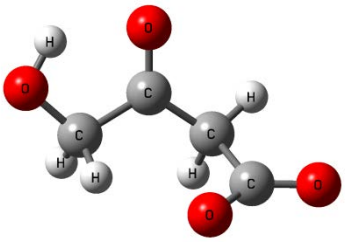
$CH_2C(O^-)CH_2C(O)OH$



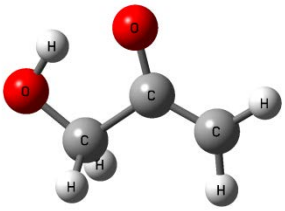
$CH_3C(O)CH_2C(O)O^-$



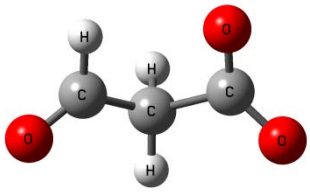
$CH_3C(O^-)CH_2$



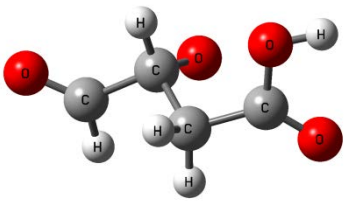
$HOCH_2C(O)CH_2C(O)O^-$



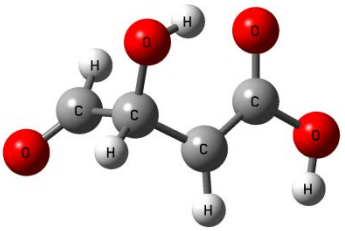
$HOCH_2C(O^-)CH_2$



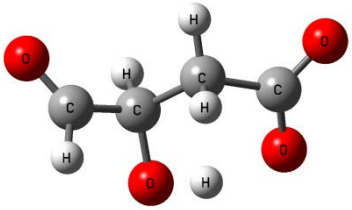
OCHCH2C(O)O-



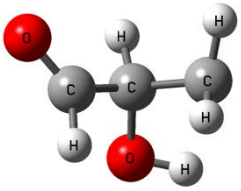
$OCHCH(O^-)CH_2C(O)OH$



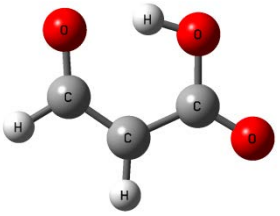
$OCHCH(OH)CHC(O^-)OH$



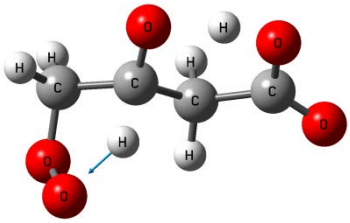
$OCHCH(OH)CH_2C(O)O^-$



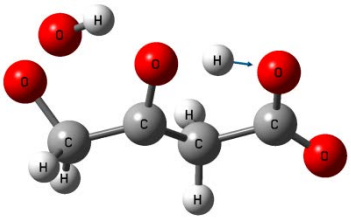
$OCHCH(OH)CH_2^-$



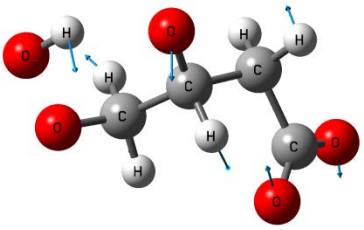
$OCHCHC(O^-)OH$



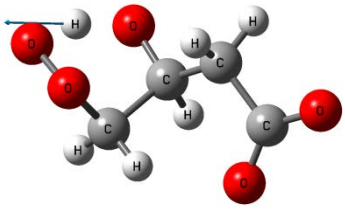
TS1



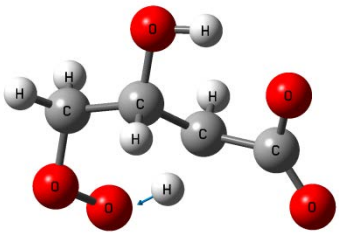
TS2



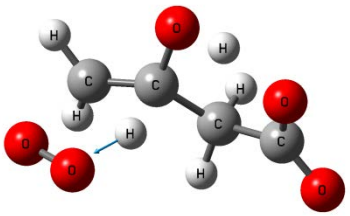
TS3



TS4



TS5



TS6

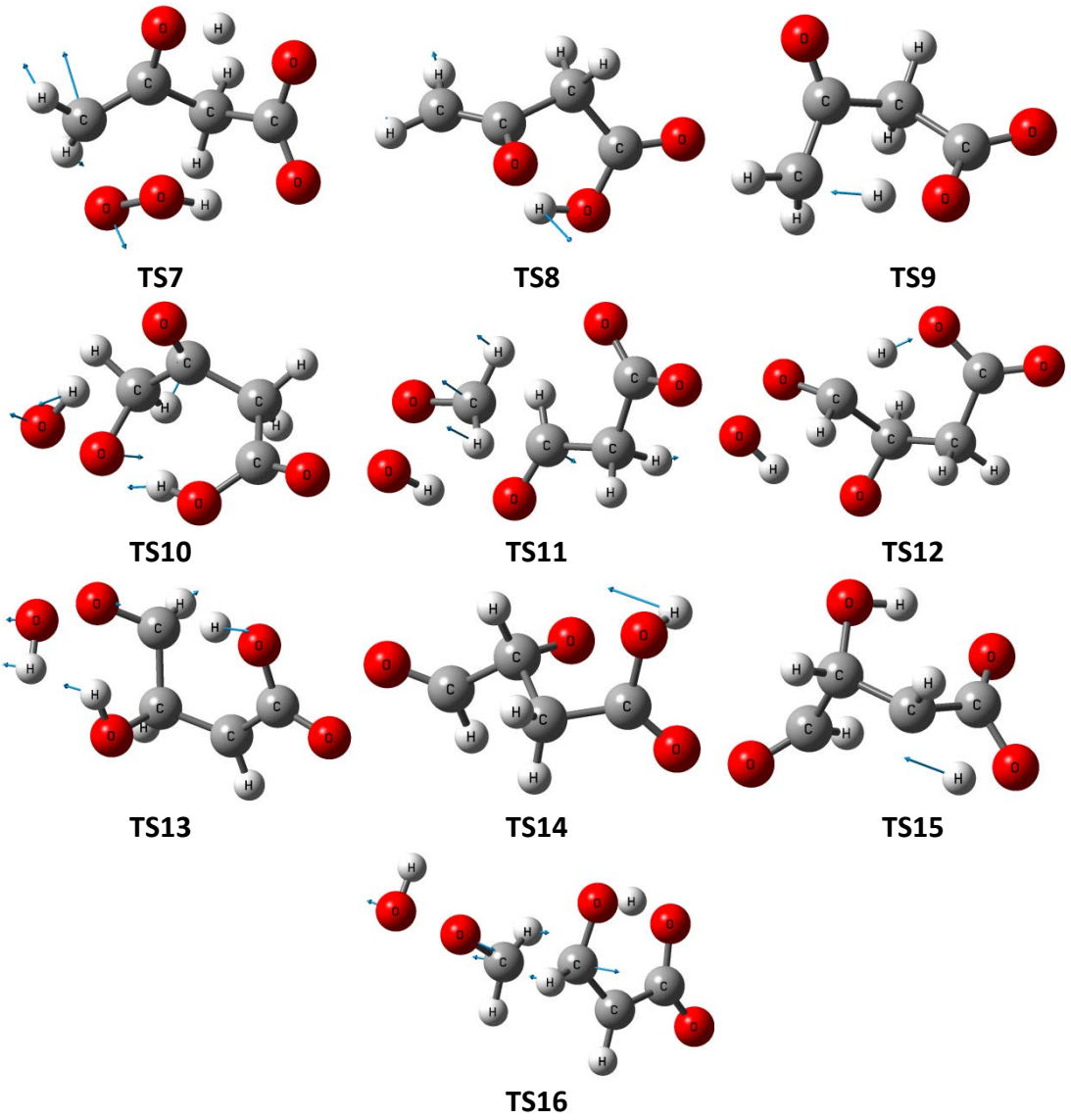


Figure S2: Optimised structures for wells (W*n*), product ions, and transition states (TS*n*) in the $^{\bullet}CH_2CH(OH)CH_2C(O)O^-$ + O_2 reaction system, at the M06-2X level of theory. Displacement vectors for imaginary frequencies of the transition states are shown.

Optimised Geometries – M06-2X/6-31G(2df,p), Å

W1			
C	4.299726	0.547023	2.092743
H	5.181019	-0.059872	2.313791
H	4.299095	0.860674	1.045079
C	3.024941	-0.224273	2.410946
H	3.022003	-0.392856	3.505497
C	1.760693	0.547431	2.028334
H	1.860706	0.866441	0.980805
H	1.633423	1.442848	2.641098
C	0.470971	-0.326705	2.115675
O	-0.577647	0.240079	2.413609
O	0.644158	-1.551121	1.828690
O	3.126983	-1.418994	1.699617
H	2.141165	-1.690516	1.645090
O	4.401770	1.767188	2.852726
O	4.829108	1.544770	4.055270

W2			
C	1.692649	0.854542	0.424249
H	2.250336	1.198203	-0.457017
H	2.157244	1.277867	1.328582
C	0.264142	1.261920	0.277179
C	-0.809545	0.487811	0.977842
H	-1.577651	1.159601	1.383055
H	-0.378584	-0.119056	1.775500
C	-1.475837	-0.409594	-0.108664
O	-2.164115	0.227721	-0.939058
O	-1.184897	-1.623712	-0.109078
O	-0.087377	1.869449	-0.885087
H	0.530568	-1.475935	-0.302093
O	1.896132	-0.540135	0.630139
O	1.463992	-1.229215	-0.530238
H	-0.981500	1.501821	-1.106090

W3			
C	1.708757	-0.861767	-0.709451
H	1.639451	-1.891549	-0.322314
H	2.097011	-0.905234	-1.739330
C	0.377962	-0.184916	-0.604837
H	-0.908873	1.332743	-0.304432
C	-0.715077	-0.861701	0.195794
H	-0.450461	-0.867419	1.272423
H	-0.871205	-1.905558	-0.087059
C	-2.064156	-0.137125	0.110588
O	-3.115700	-0.722288	0.267260
O	-1.966735	1.150091	-0.100322
O	0.397080	1.140393	-0.566100
H	1.600280	0.961550	0.869435
O	2.759581	-0.146619	-0.045064
O	2.266019	0.322188	1.200543

W4			
C	-4.677251	3.561374	0.552547
H	-4.723916	3.758596	1.632649
H	-5.253870	2.667954	0.306761
C	-5.238080	4.749687	-0.235237
C	-6.571867	5.241510	0.419619
H	-6.917638	6.137575	-0.100058
H	-6.400548	5.497702	1.467475
C	-7.730034	4.128196	0.310927
O	-8.704947	4.476774	0.982497
O	-7.496488	3.152364	-0.404081
O	-4.460331	5.843273	-0.207488
H	-2.957806	5.108176	0.480352
O	-3.334784	3.296597	0.191593
O	-2.519644	4.292706	0.798897
H	-5.520168	4.430718	-1.253341

W5			
C	2.078395	-0.055723	0.228042
H	2.545654	0.861590	-0.143669
H	2.066784	-0.043136	1.325159
C	0.657092	-0.109423	-0.344294
H	0.780421	-0.512176	-1.378324
C	-0.278733	-1.007193	0.417073
H	0.099475	-1.839821	1.000967
H	1.708950	-2.511707	-0.172118
C	-1.767266	-0.804859	0.371973
O	-2.468769	-1.710565	0.836783
O	-2.147361	0.290557	-0.153237
O	0.175256	1.202971	-0.384504
H	-0.832698	1.056441	-0.335128

$^{\bullet}CH_2CH(OH)CH_2C(O)O^-$			
C	2.432663	4.880036	0.212840
H	2.931017	4.059657	-0.291233
H	1.367541	5.011161	0.053321
C	3.076489	5.457796	1.422627
H	2.778189	6.524998	1.498414
C	2.569492	4.771731	2.712326
H	2.793698	3.700033	2.626235
H	1.486711	4.880864	2.821016
C	3.268124	5.310450	4.000345
O	2.595983	5.327091	5.033167
O	4.476152	5.654101	3.846787
O	4.466476	5.333466	1.325862
H	4.736786	5.465584	2.285847

TS1			
C	-15.959248	-2.186906	-0.010286
H	-15.361881	-1.343654	-0.383827
H	-15.993786	-2.184453	1.087462
C	-17.351484	-2.097890	-0.680706
H	-16.855009	-2.657257	-1.678690
C	-18.349868	-3.128077	-0.112062
H	-18.446712	-2.947754	0.969527
C	-19.762938	-2.998779	-0.684737
O	-20.528419	-3.935947	-0.724263
O	-20.077786	-1.785476	-1.074817
O	-17.831772	-0.891669	-0.855864
H	-19.176205	-1.216995	-1.005374
O	-15.435208	-3.419567	-0.420108
O	-15.565372	-3.401532	-1.804031
H	-17.996354	-4.150835	-0.243483

TS2			
C	1.601104	-0.537455	0.661298
H	1.657248	-0.069328	1.656711
H	1.997784	-1.562011	0.735303
C	0.197292	-0.481517	0.156739
H	-1.093975	-0.338664	-1.260647
C	-0.828574	0.362524	0.871809
H	-0.554203	1.433224	0.801928
H	-0.893755	0.133630	1.938471
C	-2.243262	0.251460	0.260159
O	-3.222084	0.492635	0.946003
O	-2.256055	-0.065736	-0.991563
O	0.059202	-0.569011	-1.170883
H	1.279679	0.947575	-1.244201
O	2.547513	0.064971	-0.231007
O	2.007399	1.293231	-0.691076

TS3			
C	0.886033	-0.673660	0.525171
H	1.039147	-0.357830	1.566622
H	0.245117	-1.559118	0.493374
C	0.210674	0.437998	-0.287543
H	-0.212005	-0.066632	-1.207230
C	-1.098149	0.911028	0.353039
H	-1.440369	1.809028	-0.171296
H	-0.967039	1.168925	1.408926
C	-2.198623	-0.204146	0.173608
O	-3.154502	-0.132272	0.950304
O	-1.960342	-1.003995	-0.759428
O	1.031060	1.426415	-0.674037
H	2.673610	0.708633	-0.184273
O	2.125552	-1.061021	-0.030894

TS4			
C	-1.136125	-0.440452	0.000000
H	-0.518982	-0.665993	0.873977
H	-2.004525	-1.085984	-0.138777
C	-1.755543	1.050620	0.224785
O	-0.718172	1.907677	0.171751
H	0.199856	1.290007	-0.444526
O	-0.370100	-0.385257	-1.140982
O	0.730732	0.402970	-0.885118
C	-2.878420	1.277493	-0.779062
H	-3.143590	2.338566	-0.774271
H	-2.521794	1.049296	-1.790099
H	-2.161827	0.933349	1.244315
C	-4.163658	0.425561	-0.480371
O	-5.184434	0.805496	-1.064111
O	-3.997449	-0.540518	0.301707

TS5			
C	-1.126146	-0.210706	0.114285
H	-0.550799	0.521931	-0.461115
H	-0.910591	-0.095260	1.185378
C	-2.623951	-0.060031	-0.138128
H	-2.786712	-0.185392	-1.220912
C	-3.362931	-1.159790	0.590467
H	-3.303072	-0.990395	1.673075
H	-2.482465	-2.143451	0.440747
C	-4.821921	-1.365110	0.123088
O	-5.291529	-2.481093	-0.055937
O	-5.357455	-0.224474	0.022205
O	-3.050653	1.214336	0.285540
H	-4.020440	1.085297	0.292391
O	-0.714464	-1.480181	-0.343821
O	-1.289356	-2.445728	0.483858

TS6			
C	-10.437986	0.030542	0.525264
H	-9.893246	0.966406	0.567022
H	-9.938064	-0.852647	0.904819
C	-11.819231	0.020747	0.326322
H	-11.608528	-0.406256	-0.866973
C	-12.687738	-1.084322	0.929697
H	-12.828351	-0.872073	1.997443
C	-14.110462	-1.168388	0.294772
O	-14.702719	-2.238767	0.412080
O	-14.518688	-0.098650	-0.249064
O	-12.462618	1.234196	0.220322
H	-13.403650	0.918872	-0.023817
O	-9.714593	-0.339974	-1.375401
O	-10.769468	-0.614128	-1.986056
H	-12.204024	-2.060564	0.846540

TS7			
C	1.728835	1.147246	0.220695
H	2.333962	1.603060	-0.554679
H	2.183834	1.025865	1.195795
C	0.360975	1.292271	0.137806
C	-0.562496	0.631897	1.118122
H	-1.195265	1.378102	1.615165
H	0.000877	0.058252	1.853429
C	-1.505020	-0.297666	0.288488
O	-2.200308	0.333414	-0.556984
O	-1.442232	-1.514966	0.484264
O	-0.218152	1.813186	-0.938777
H	0.380964	-1.517328	-0.399982
O	2.054957	-0.727519	-0.089583
O	1.119515	-1.235960	-0.970813
H	-1.153259	1.389780	-0.942654

TS8			
C	-1.622857	0.916769	0.099529
H	-2.565556	1.254361	-0.317106
H	-0.846996	1.652268	0.271996
C	-1.458861	-0.395494	0.467474
C	-0.060216	-0.776174	0.999280
H	-0.150951	-1.358926	1.920159
C	0.696797	-1.647985	0.008051
O	0.257606	-1.599821	-1.257946
O	1.662295	-2.312483	0.286326
O	-2.242728	-1.375370	0.332296
H	0.579631	0.089537	1.206810
H	-0.570926	-1.091834	-1.257172

TS9			
C	-1.487283	1.145749	0.256185
H	-2.415717	1.521419	-0.168848
H	-1.242753	1.560058	1.235545
C	-1.267016	-0.266260	0.115592
C	0.089714	-0.698464	0.685936
H	0.234161	-1.773691	0.581874
C	1.275460	0.025055	-0.003147
O	1.008305	1.196122	-0.488476
O	2.369315	-0.509690	-0.033165
O	-1.931018	-1.066856	-0.538695
H	0.154948	-0.434751	1.748759
H	-0.136846	1.364569	-0.321610

TS10			
C	-10.297732	5.016085	-0.010747
H	-9.302009	5.419971	-0.240417
H	-10.522748	5.115844	1.058522
C	-11.335734	5.596093	-0.885248
H	-11.768046	3.239783	-0.745426
C	-12.781736	5.431972	-0.459849
H	-13.397056	6.271894	-0.795305
H	-12.863806	5.356904	0.632197
C	-13.449046	4.170967	-1.029905
O	-14.597317	4.159694	-1.401401
O	-12.705697	3.074880	-1.056640
O	-11.060916	5.878742	-2.080619
H	-9.962587	4.085331	-2.168126
O	-10.230009	3.580749	-0.264326
O	-9.485731	3.379309	-1.695838

TS11			
C	-6.727089	3.741688	0.000000
H	-6.730043	4.048542	1.043462
H	-7.521219	3.127968	-0.426062
C	-7.420509	5.573640	-0.901089
C	-8.808449	5.728367	-0.339149
H	-9.292894	6.513907	-0.941808
H	-8.764030	6.121285	0.682042
C	-9.782288	4.477738	-0.424987
O	10.834309	4.612379	0.217498
O	-9.391275	3.523819	-1.145009
O	-6.464621	6.335733	-0.590805
H	-5.109919	5.394524	-0.364243
O	-5.520185	3.567444	-0.568007
O	-4.600638	4.581103	-0.076776
H	-7.388641	5.008072	-1.849515

TS12			
C	-0.807334	-0.747445	-0.406209
H	-1.018211	-0.770717	-1.483766
H	0.350515	-1.293496	-0.050121
C	-0.247606	0.730677	-0.048106
C	1.156382	0.808810	-0.656041
H	1.598182	1.791371	-0.478099
H	1.061231	0.684093	-1.742454
C	2.130487	-0.257753	-0.112552
O	3.313515	0.017863	0.000131
O	1.600060	-1.399966	0.172586
O	-1.179836	1.514801	-0.557093
H	-2.683161	0.528543	-0.325316
O	-1.918465	-1.037235	0.328608
O	-3.062031	-0.377192	-0.244764
H	-0.192145	0.715645	1.058587

TS13			
C	0.695021	-0.724508	-0.620928
H	-0.723064	-1.387312	-0.280173
H	0.798221	-0.618926	-1.710971
C	0.302456	0.604351	0.046202
C	-1.163408	0.879769	-0.106432
C	-2.203340	-0.165883	-0.036108
O	-1.784045	-1.413333	-0.084958
O	-3.381342	0.138210	0.058169
O	0.625898	0.522579	1.439254
H	2.839002	0.164455	0.586104
O	1.706566	-1.334645	-0.010171
O	3.073852	-0.471754	-0.100155
H	-1.540905	1.896447	-0.113036
H	0.922286	-0.393540	1.540258
H	0.872161	1.458428	-0.357011

TS14			
C	1.846927	-0.764779	-0.001878
H	1.633546	-1.829798	0.267507
C	0.585634	0.071320	0.144873
C	-0.450363	-0.367465	-0.981054
H	-0.339756	-1.421876	-1.252317
H	-0.385054	0.262164	-1.874878
C	-1.766867	-0.202468	-0.289965
O	-1.997764	1.108390	0.040338
O	-2.541090	-1.069234	-0.000271
O	0.131359	-0.172578	1.371410
O	2.977315	-0.390513	-0.207361
H	-2.149828	1.081786	0.992185
H	0.868627	1.127270	-0.096965

TS15			
C	-1.542751	-0.859858	0.120177
H	-1.144164	-0.960870	-0.917580
C	-0.916184	0.300320	0.858948
C	0.549823	-0.023453	1.032281
H	1.001138	0.620711	1.795523
C	1.356400	0.103701	-0.239195
O	2.263635	-0.839940	-0.123185
O	1.195063	0.846793	-1.204107
O	-1.169648	1.482450	0.100794
H	-0.411703	1.541249	-0.508022
O	-2.376359	-1.620773	0.541749
H	1.535361	-1.088400	0.813172
H	-1.433365	0.395757	1.821368

TS16			
C	1.109557	-0.569441	-0.489997
H	0.630125	-1.348878	0.112283
H	0.993831	-0.701714	-1.572251
C	-0.078485	0.854709	0.098283
C	-1.183911	0.459370	-0.693970
H	-1.200723	0.678473	-1.754948
H	3.301442	-1.552642	0.771770
C	-2.238994	-0.445584	-0.124572
O	-3.160555	-0.802936	-0.855962
O	-2.054304	-0.751869	1.107703
O	-0.144308	0.720114	1.422431
H	-0.969220	0.051993	1.510968
O	2.248044	-0.088871	-0.072769
O	3.418275	-1.304672	-0.152459
H	0.544037	1.681828	-0.246092

Vibrational Frequencies – M06-2X/6-31G(2df,p), cm^{-1}

W1	W2	W3	W4	W5
60.31	75.75	49.52	57.26	53.63
71.44	93.81	85.53	76.43	83.05
96.48	141.61	111.25	128.75	114.09
128.92	210.58	191.32	187.37	143.00
189.05	228.30	231.52	221.20	237.87
309.04	278.80	265.89	266.96	315.09
395.20	361.89	387.54	348.23	357.70
414.24	401.20	423.66	354.11	387.48
438.76	439.92	437.80	443.68	394.51
495.77	477.11	509.73	485.13	430.12
586.06	585.31	580.30	596.16	498.11
634.02	639.45	661.77	607.38	537.48
764.19	767.68	750.98	620.08	645.22
877.65	807.25	760.76	668.88	757.43
913.20	870.77	881.92	795.73	766.10
932.24	878.76	911.25	851.75	893.38
985.99	909.90	929.20	910.26	962.47
1025.53	918.51	956.82	946.70	994.68
1071.02	973.81	985.34	978.36	1002.40
1110.76	1025.09	1059.08	1057.31	1036.69
1171.77	1087.50	1132.12	1121.16	1079.86
1218.43	1122.00	1186.10	1141.93	1125.86
1241.99	1204.63	1230.74	1156.66	1193.30
1269.72	1254.41	1242.65	1186.03	1246.56
1304.16	1275.23	1267.39	1248.30	1275.64
1337.23	1334.61	1308.59	1288.58	1312.73
1358.39	1380.89	1377.50	1323.29	1336.26
1379.83	1437.38	1442.82	1364.21	1382.36
1418.01	1454.43	1454.81	1410.01	1408.25
1454.77	1461.71	1472.24	1452.13	1447.86
1475.50	1519.40	1527.63	1464.16	1464.19
1600.26	1574.03	1714.93	1551.84	1603.20
1808.67	1744.19	1778.83	1825.04	1757.73
2745.51	3006.19	1985.38	2995.45	2777.26
2966.11	3020.82	2925.67	3041.55	2851.53
3028.32	3077.56	2990.24	3092.21	3056.71
3090.00	3140.41	3026.86	3159.50	3126.14
3119.60	3253.10	3101.61	3173.70	3204.70
3162.44	3305.28	3526.25	3516.09	3767.77

TS1	TS2	TS3	TS4
-958.96	-507.93	-138.58	-1389.55
80.05	53.38	66.81	41.40
87.53	91.25	91.95	93.90
150.70	106.81	142.42	142.33
211.53	215.77	236.79	220.84
342.44	233.01	256.77	272.78
392.46	275.56	359.39	353.51
417.24	398.66	375.35	425.24
466.05	427.59	450.46	477.58
538.04	446.83	478.91	522.86
577.01	576.37	583.87	571.59
631.92	639.14	626.40	629.41
668.80	694.42	635.74	675.02
713.16	728.09	699.55	700.24
882.19	844.69	826.08	720.28
906.00	884.26	855.68	881.46
947.86	927.42	935.67	906.26
1003.80	937.04	947.86	953.31
1039.31	958.16	969.31	984.88
1090.41	991.80	1029.99	995.55
1124.09	1062.97	1059.24	1044.26
1181.96	1136.55	1123.22	1091.03
1193.59	1199.55	1135.62	1139.18
1248.68	1244.09	1170.03	1189.12
1250.03	1288.29	1213.19	1221.13
1281.09	1311.92	1272.38	1243.42
1289.29	1380.63	1295.75	1270.98
1322.11	1437.74	1349.72	1299.47
1439.75	1441.29	1386.50	1371.33
1459.50	1454.52	1455.41	1399.20
1475.79	1469.61	1461.51	1455.43
1710.65	1543.38	1535.16	1482.70
1820.24	1820.09	1782.01	1783.03
1825.18	1890.66	2626.63	1837.82
2130.66	2939.19	3040.89	2988.10
3017.07	2997.51	3066.08	3064.86
3025.08	3036.60	3122.96	3083.49
3088.59	3099.94	3148.23	3122.74
3149.49	3618.92	3610.36	3212.14

TS5	TS6	TS7	TS8
-1729.20	-906.32	-540.48	-213.33
64.11	62.38	81.68	71.91
125.98	72.29	97.54	206.99
163.75	131.59	120.01	393.64
225.85	173.00	163.06	400.74
297.28	268.78	182.07	474.68
346.88	299.61	296.87	544.64
370.35	365.08	357.53	583.05
437.73	403.63	386.55	591.90
455.83	487.02	435.20	610.90
546.92	527.66	512.12	701.06
599.22	533.74	556.87	768.80
654.84	639.51	639.34	877.54
756.56	747.83	763.05	906.09
784.22	788.99	805.96	946.08
897.35	842.59	881.51	1049.97
956.39	908.17	893.97	1170.67
976.03	933.77	916.29	1250.77
987.49	955.95	923.40	1277.10
1075.82	1001.61	977.33	1335.70
1121.33	1041.36	1016.02	1433.32
1124.47	1059.68	1033.58	1441.91
1168.43	1190.02	1063.96	1481.39
1229.26	1237.30	1138.37	1703.65
1265.49	1255.32	1217.64	1884.00
1285.56	1274.49	1296.29	3062.87
1304.29	1384.10	1395.01	3119.13
1352.26	1410.83	1439.06	3150.42
1374.42	1438.44	1448.98	3240.03
1395.86	1450.48	1489.08	3708.79
1478.33	1525.57	1566.67	
1480.17	1566.63	1633.14	
1589.32	1642.42	1791.06	
1794.14	1811.44	2690.31	
3013.13	2794.80	3034.25	
3042.63	3045.97	3148.07	
3076.80	3126.47	3164.34	
3114.23	3159.95	3260.00	
3544.78	3257.78	3656.35	

TS9	TS10	TS11	TS12
-880.77	-1979.53	-314.83	-1256.36
95.02	67.59	34.41	69.59
136.50	82.54	82.30	141.87
392.49	108.40	111.20	147.10
424.12	154.74	169.39	196.14
464.76	212.08	225.82	301.18
552.12	272.04	255.58	331.30
599.97	318.14	277.86	391.81
631.21	407.44	379.33	423.92
678.40	416.22	422.15	460.35
769.23	539.27	500.08	510.45
853.17	557.67	530.80	636.64
918.06	587.90	561.81	643.24
932.24	631.18	626.71	658.49
970.92	723.78	724.69	681.93
1066.10	810.23	746.68	773.54
1151.32	884.72	846.37	913.91
1227.87	897.07	873.86	932.85
1291.41	930.02	892.47	936.93
1353.67	984.44	979.62	1031.99
1411.81	1034.28	1027.22	1073.72
1448.43	1119.49	1077.38	1135.48
1468.13	1159.92	1169.11	1159.29
1693.28	1245.95	1192.36	1212.22
1778.34	1284.11	1214.30	1254.56
1853.62	1294.00	1244.91	1296.15
3052.89	1305.46	1346.71	1316.30
3098.26	1336.22	1400.16	1399.17
3152.65	1435.42	1427.97	1407.35
3187.25	1453.67	1475.06	1425.69
	1470.11	1557.41	1464.02
	1567.83	1638.79	1557.25
	1864.91	1800.54	1673.65
	2975.07	3023.78	1819.40
	3025.16	3035.83	2950.38
	3040.49	3108.37	3055.53
	3089.83	3127.79	3074.92
	3103.33	3268.15	3128.16
	3648.47	3285.43	3411.39

TS13	TS14	TS15	TS16
-375.17	-463.04	-1646.95	-1078.21
77.31	62.28	74.25	62.88
81.21	73.19	90.88	73.09
128.30	150.90	151.78	111.87
162.97	225.97	233.25	113.98
303.34	303.23	325.81	184.52
330.27	334.40	378.62	218.01
364.79	404.46	395.78	246.28
392.44	419.37	521.43	282.16
437.98	497.82	570.51	323.74
512.65	611.12	660.61	386.43
536.33	727.69	680.08	437.02
569.73	816.64	792.08	512.61
611.10	889.81	857.89	623.59
687.87	934.22	904.00	670.91
723.28	1001.67	1026.96	807.33
786.87	1069.81	1055.59	818.56
855.60	1110.40	1078.43	875.27
897.24	1212.97	1158.42	936.73
961.66	1215.67	1204.12	981.66
1071.14	1244.68	1278.24	1043.86
1092.65	1301.47	1304.07	1048.67
1180.30	1328.43	1327.52	1123.49
1201.21	1369.50	1402.47	1173.25
1228.64	1409.66	1429.47	1226.53
1257.73	1453.65	1516.04	1239.48
1297.08	1836.87	1715.23	1262.16
1343.66	1893.57	1872.80	1318.79
1375.40	2811.02	2115.60	1355.78
1387.64	2882.20	2893.39	1443.47
1451.93	3051.36	3057.76	1532.93
1609.54	3119.79	3081.91	1612.79
1736.39	3857.93	3608.58	1790.01
1973.46			2253.43
2983.21			3034.48
3017.42			3122.80
3205.41			3130.11
3752.96			3210.19
3832.64			3863.22