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SUPPORTING INFORMATION

Theoretical Investigation on Unimolecular Decomposition of Malonic Acid: A Potential Sink for Ketene

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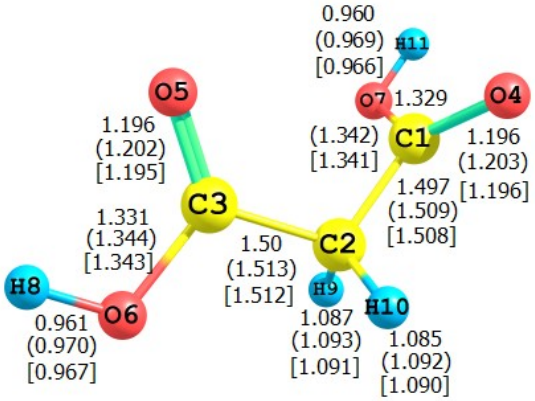
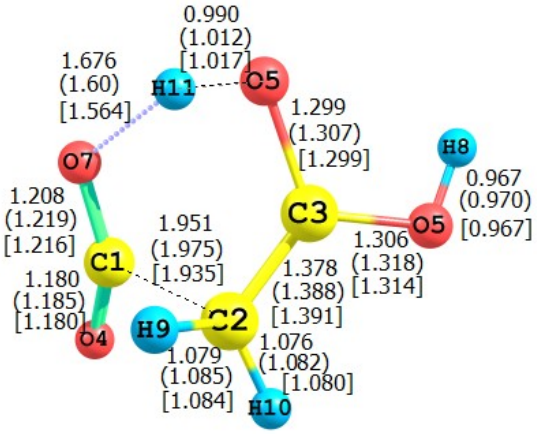
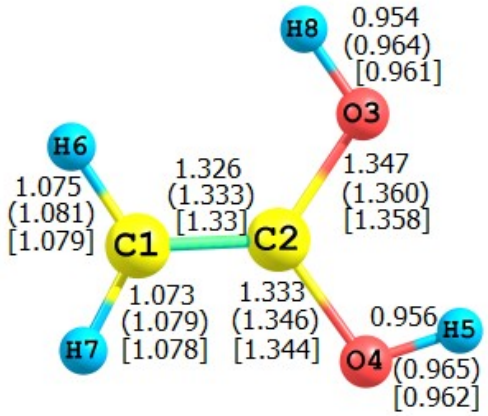


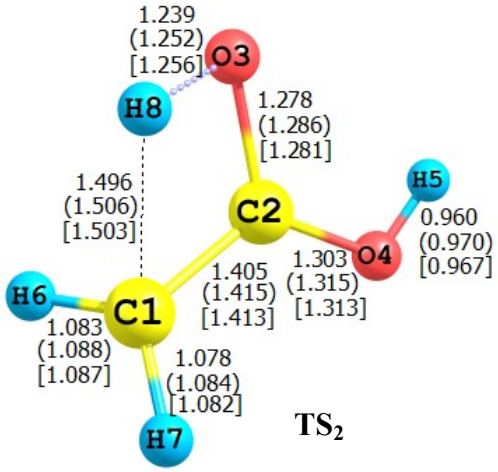
$CH_2(COOH)_2$



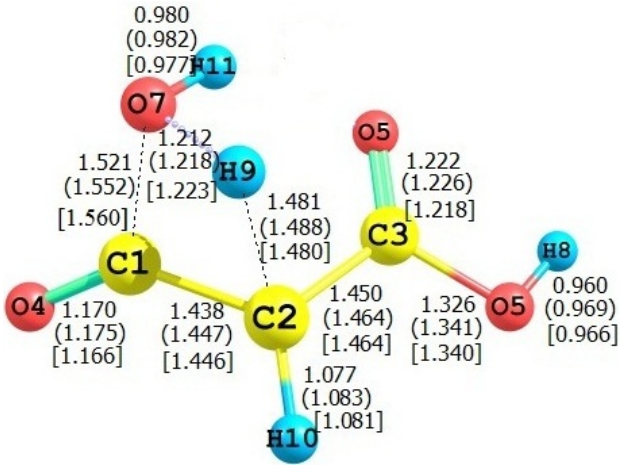
TS_1



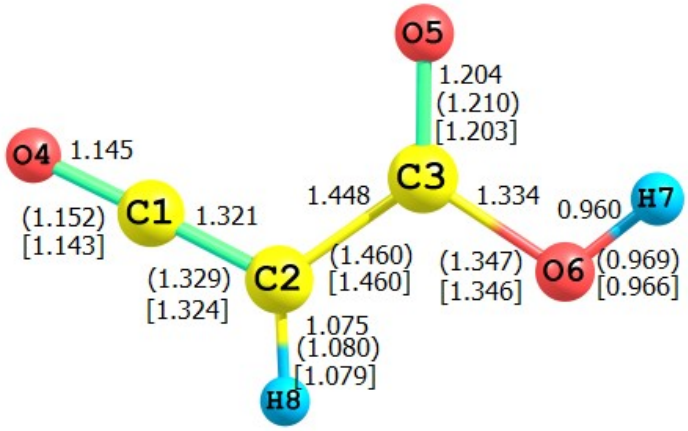
$CH_2C(OH)_2$



TS_2



TS_3



COCHC(O)OH

Continue…

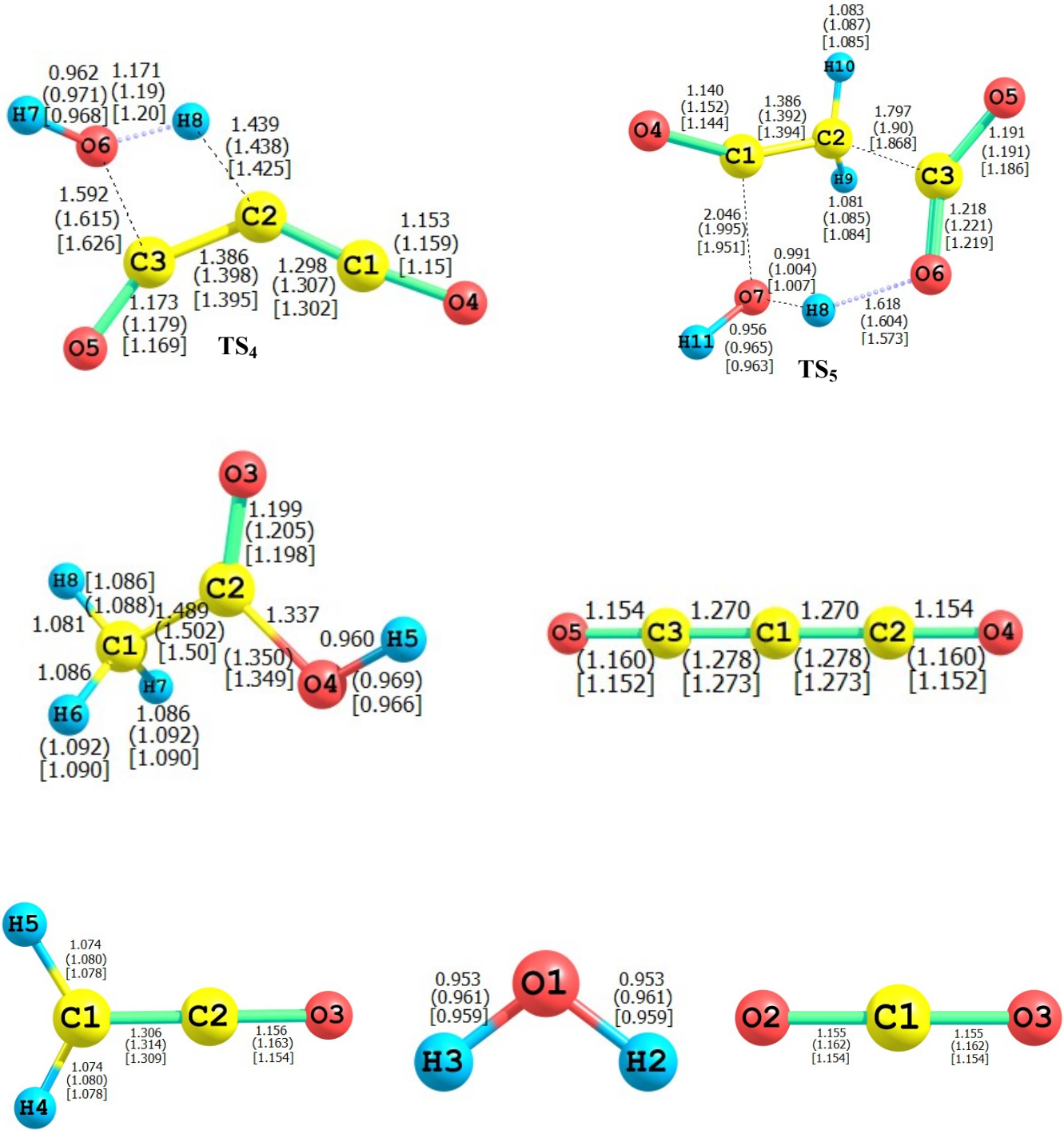


Fig. S1 Optimized geometries of reactant, transition states, intermediates and products involved in the unimolecular decomposition of malonic acid at MPWB1K/6-31+G(d,p), M06-2X/6-31+G(d,p) (in parentheses) and M06-2X/6-311++G(d,p) (in square bracket) levels . Bond lengths are in angstroms.

Table S1. Harmonic vibrational frequency of reactant, transition states, intermediates and products involved in the unimolecular decomposition of malonic acid at MPWB1K/6-31+G(d,p), M06-2X/6-31+G(d,p) (in parentheses) and M06-2X/6-311++G(d,p) (in square bracket) levels

Species	Vibrational Frequencies (cm^{-1})
$CH_2(COOH)_2$	43, 72, 165, 374, 411, 533, 549, 615, 650, 680, 770, 938, 961, 986, 1195, 1219, 1268, 1315, 1428, 1467, 1485, 1924, 1937, 3169, 3235, 3912, 3919 (48, 68, 160, 373, 408, 521, 543, 612, 641, 659, 756, 919, 938, 968, 1171, 1192, 1253, 1292, 1394, 1430, 1458, 1890, 1905, 3111, 3172, 3827, 3831) [50, 71, 161, 374, 411, 528, 547, 618, 644, 663, 762, 920, 936, 970, 1170, 1191, 1257, 1297, 1386, 1421, 1456, 1887, 1904, 3097, 3155, 3835, 3837]
TS1	399i, 88, 134, 288, 359, 454, 554, 576, 607, 690, 747, 829, 874, 938, 1050, 1068, 1230, 1304, 1380, 1478, 1582, 1726, 2153, 3245, 3356, 3361, 3909 (455i, 92, 135, 267, 363, 452, 550, 573, 604, 680, 732, 858, 870, 916, 1030, 1047,1208, 1278, 1373, 1454, 1540, 1691, 2108, 2992, 3182, 3288, 3815) [484i, 93, 137, 286, 372, 455, 557, 584, 614, 692, 748, 866, 907, 927, 1028, 1059, 1204, 1283, 1383, 1455, 1535, 1680, 2082, 2861, 3156, 3264, 3817]
$CH_2C(OH)_2$ (IM1)	180, 370, 458, 542, 672, 707, 780, 982, 1006, 1213, 1249, 1463, 1483, 1833, 3279, 3385, 3975, 3999 (182, 357, 451, 538, 656, 688, 763, 958, 982, 1193, 1232, 1431, 1449, 1802, 3214, 3314, 3878, 3907) [161, 342, 453, 543, 661, 687, 751, 955, 979, 1197, 1239, 1432, 1440, 1789, 3193, 3295, 3892, 3910]
TS2	2167i, 426, 500, 570, 642, 769, 827, 1043, 1092,1187, 1241, 1453,1602, 1659, 2079, 3213, 3313, 3911 (2103i, 418, 504, 567, 632, 754, 809, 1021, 1073, 1161, 1218, 1430, 1561, 1629, 2038, 3165, 3261, 3828) [2120i, 419, 505, 570, 630, 756, 804, 1018, 1074, 1151, 1228, 1425, 1549, 1620, 2020, 3148, 3243, 3833]
TS3	1796i, 117, 140, 251, 407, 480, 562, 569, 611, 663, 702, 797, 851, 880, 1015, 1160, 1172, 1235, 1312, 1479, 1511, 1807, 1908, 2081, 3308, 3611, 3917 (1708i, 110, 137, 231, 398, 462, 528, 547, 588, 640, 689, 770, 823, 857, 991, 1113, 1132, 1200, 1285, 1440, 1465, 1776, 1865, 2049, 3242, 3638, 3823) [1742i, 105, 134, 219, 398, 460, 516, 541, 574, 638, 689, 769, 816, 856, 986, 1097, 1125, 1194, 1288, 1433, 1454, 1771, 1852, 2050, 3228, 3667, 3835]
COCHCOOH (IM2)	114, 138, 419, 528, 532, 590, 627, 710, 803, 991, 1139, 1215, 1353, 1526, 1871, 2333, 3329, 3928 (111, 139, 415, 524, 530, 577, 623, 699, 783, 970, 1114, 1189, 1325, 1483, 1835, 2292, 3268, 3820) [110, 140, 418, 525, 530, 592, 613, 705, 788, 966, 1109, 1185, 1326, 1471, 1832, 2291, 3252, 3835]
TS4	1676i, 115, 127, 385, 485, 577, 587, 632, 642, 781, 941, 1014, 1239, 1555, 1989, 2100, 2314, 3896 (1590i, 115, 125, 383, 492, 565, 578, 619, 627, 769, 929, 996, 1227, 1520, 1940, 2059, 2272, 3804) [1633i, 108, 124, 377, 464, 571, 583, 617, 631, 771, 916, 982, 1199, 1514,

	1928, 2062, 2274, 3813]
TS5	336i, 63, 115, 219, 275, 310, 397, 460, 489, 614, 632, 659, 748, 854, 955, 1015, 1071, 1115, 1350, 1455, 1671, 2060, 2261, 3207, 3270, 3305, 3997 (410i, 69, 110, 178, 279, 302, 381, 463, 490, 607, 625, 657, 717, 812, 945, 962, 1066, 1084, 1316, 1435, 1631, 2065, 2192, 3089, 3161, 3264, 3907) [416i, 70, 111, 212, 291, 323, 392, 478, 501, 616, 643, 683, 734, 829, 965, 988, 1059, 1098, 1311, 1435, 1623, 2038, 2181, 2976, 3138, 3235, 3894]
CH_3COOH	63, 427, 558, 600, 687, 909, 1030, 1090, 1253, 1380, 1463, 1499, 1506, 1921, 3146, 3227, 3276, 3916 (105, 429, 548, 594, 665, 889, 1014, 1075, 1230, 1354, 1434, 1481, 1484, 1885, 3096, 3176, 3208, 3836) [126, 432, 548, 601, 663, 887, 1016, 1079, 1234, 1351, 1429, 1479, 1482, 1885, 3087, 3164, 3192, 3839]
C_3O_2	159(2), 621(2), 716(2), 811,1719,2367,2466 (168(2), 615(2), 725(2), 801, 1699, 2338, 2431) [77(2), 618(2), 627(2), 797, 1698, 2337, 2424]
CH_2CO	449, 568, 635, 1011, 1209, 1450, 2307, 3285, 3391 (440, 558, 624, 994, 1187, 1425, 2268, 3221, 3325) [449, 578, 619, 993, 1184, 1416, 2269, 3206, 3311]
CO_2	687, 687, 1434, 2516 (676, 676, 1414, 2469) [690, 690, 1419, 2472]
H_2O	1636, 3974, 4100 (1596, 3887, 4012) [1595,3894,4000]

Table S2. Total energies (hartee), ZPE (hartee/particle), corrected total energies and T1 diagnostic values of reactant, transition states, intermediates and products involved in the unimolecular decomposition of malonic acid at CCSD(T)//M06-2X/6-311++G(d,p) level.

Species	Total energy	ZPE	Scaling Factor	Corrected ZPE	Corrected total energy	T1 diag
$CH_2(COOH)_2$	-416.8177239	0.078737	0.967	0.076138679	-416.7415852	0.016
TS1	-416.763151	0.075315	0.967	0.072829605	-416.6903214	0.019
$CH_2C(OH)_2$ (IM1)	-228.5663445	0.061332	0.967	0.059308044	-228.5070365	0.012
TS2	-228.4903581	0.056956	0.967	0.055076452	-228.4352816	0.017
TS3	-416.7044548	0.072243	0.967	0.069858981	-416.6345958	0.017
COCHCOOH (IM2)	-340.4819966	0.049431	0.967	0.047799777	-340.4341968	0.018
TS4	-340.3763674	0.04315	0.967	0.04172605	-340.3346414	0.019
TS5	-416.7404044	0.072535	0.967	0.070141345	-416.6702631	0.019
CH_3COOH	-228.6133363	0.062655	0.967	0.060587385	-228.5527489	0.015
C_3O_2	-264.1591433	0.022565	0.967	0.021820355	-264.1373229	0.021
CH_2CO	-152.2672338	0.031961	0.967	0.030906287	-152.2363275	0.017
CO_2	-188.2208013	0.012013	0.967	0.011616571	-188.2091847	0.018
H_2O	-76.286542	0.021621	0.967	0.020907507	-76.26563449	0.010

Table S3. Cartesian coordinates of reactant, transition states, intermediates and products involved in the unimolecular decomposition of malonic acid at three levels of theory.

$CH_2(COOH)_2$

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.265937	-0.209912	0.028017
2	6	0	0.066576	-0.820060	0.337797
3	6	0	1.188364	0.076506	-0.096446
4	8	0	-2.002484	-0.579252	-0.839717
5	8	0	1.066872	1.095634	-0.710637
6	8	0	2.367089	-0.418389	0.276449
7	8	0	-1.546038	0.794359	0.852688
8	1	0	3.048533	0.179104	-0.043795
9	1	0	0.163490	-1.006355	1.404397
10	1	0	0.154132	-1.767254	-0.185013
11	1	0	-2.383691	1.176485	0.577947

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.271281	-0.217144	0.023262
2	6	0	0.069608	-0.832842	0.341938
3	6	0	1.192417	0.082711	-0.095298
4	8	0	-1.990079	-0.559201	-0.879137
5	8	0	1.061815	1.112928	-0.702106
6	8	0	2.386149	-0.415244	0.272303
7	8	0	-1.574294	0.767502	0.883840
8	1	0	3.069607	0.195137	-0.046108
9	1	0	0.167296	-1.016034	1.415570
10	1	0	0.164143	-1.783243	-0.187471
11	1	0	-2.414234	1.159906	0.599402

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.270379	-0.218926	0.018222
2	6	0	0.070195	-0.830839	0.340471
3	6	0	1.190485	0.087250	-0.094553
4	8	0	-1.974728	-0.546820	-0.891422
5	8	0	1.059772	1.114325	-0.692618
6	8	0	2.382551	-0.413929	0.270453
7	8	0	-1.583215	0.749751	0.891919
8	1	0	3.065294	0.195161	-0.042894
9	1	0	0.166206	-1.013175	1.412333
10	1	0	0.169965	-1.778816	-0.188336

11	1	0	-2.418311	1.145305	0.607410

TS1

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.456075	0.023082	-0.104493
2	6	0	0.087667	-0.738404	0.815500
3	6	0	1.139851	-0.122069	0.172587
4	8	0	-2.196218	-0.862517	-0.350199
5	8	0	1.260762	1.169567	0.091604
6	8	0	2.040394	-0.801804	-0.487031
7	8	0	-1.275614	1.217418	-0.124474
8	1	0	2.571619	-0.199943	-1.015830
9	1	0	-0.232456	-0.283520	1.740912
10	1	0	0.053053	-1.812928	0.769293
11	1	0	0.344539	1.539416	0.164859

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.463567	0.020927	-0.106580
2	6	0	0.097816	-0.778524	0.801408
3	6	0	1.150241	-0.123914	0.174605
4	8	0	-2.225743	-0.853927	-0.351478
5	8	0	1.238200	1.179174	0.115227
6	8	0	2.074461	-0.782020	-0.497693
7	8	0	-1.265782	1.223744	-0.118445
8	1	0	2.600215	-0.152515	-1.016144
9	1	0	-0.232336	-0.351863	1.743815
10	1	0	0.072379	-1.857339	0.718262
11	1	0	0.283713	1.515019	0.156570

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.451476	0.013996	-0.100775
2	6	0	0.082548	-0.781648	0.771779
3	6	0	1.147984	-0.120014	0.168856
4	8	0	-2.226216	-0.841591	-0.348165
5	8	0	1.224077	1.175939	0.115365
6	8	0	2.085959	-0.774079	-0.479850
7	8	0	-1.257416	1.215319	-0.113946
8	1	0	2.622582	-0.143679	-0.981019
9	1	0	-0.233506	-0.374195	1.726150
10	1	0	0.066529	-1.858265	0.679170
11	1	0	0.258833	1.497435	0.149304

$CH_2C(OH)_2$ (IM1)

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.392708	1.349242	0.000000
2	6	0	0.000000	0.082349	0.000000
3	8	0	-0.799456	-1.002591	0.000000
4	8	0	1.280465	-0.290336	0.000000
5	1	0	1.322388	-1.246062	0.000000
6	1	0	-1.437710	1.604122	0.000000
7	1	0	0.340485	2.133789	0.000000
8	1	0	-1.716984	-0.737980	0.000000

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.371426	1.364591	0.000000
2	6	0	0.000000	0.083708	0.000000
3	8	0	-0.824973	-0.998184	0.000000
4	8	0	1.286763	-0.311722	0.000000
5	1	0	1.313939	-1.276903	0.000000
6	1	0	-1.417480	1.639448	0.000000
7	1	0	0.382848	2.137309	0.000000
8	1	0	-1.745069	-0.710402	0.000000

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.382471	1.357813	0.000000
2	6	0	0.000000	0.083990	0.000000
3	8	0	-0.815648	-1.002715	0.000000
4	8	0	1.287847	-0.300550	0.000000
5	1	0	1.318111	-1.262705	0.000000
6	1	0	-1.429985	1.620021	0.000000
7	1	0	0.362996	2.136522	0.000000
8	1	0	-1.733891	-0.718541	0.000000

TS2

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.232937	-0.596739	-0.049822
2	6	0	-0.051598	-0.031758	0.034259
3	8	0	0.013574	1.243890	-0.009419
4	8	0	-1.205694	-0.637616	0.032684
5	1	0	-1.901126	0.010235	-0.108326
6	1	0	1.841680	-0.358026	0.814231
7	1	0	1.369929	-1.594565	-0.435596
8	1	0	1.138451	0.863147	-0.363049

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.244158	-0.598131	-0.049324
2	6	0	-0.048957	-0.029023	0.037029
3	8	0	0.004984	1.255893	-0.009550
4	8	0	-1.209105	-0.649467	0.033435
5	1	0	-1.913944	0.000050	-0.115755
6	1	0	1.860840	-0.360591	0.816000
7	1	0	1.374680	-1.597893	-0.447592
8	1	0	1.140189	0.869955	-0.369969

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.241264	-0.598265	-0.049789
2	6	0	-0.049573	-0.027456	0.034738
3	8	0	0.005376	1.252095	-0.009400
4	8	0	-1.207077	-0.647501	0.033335
5	1	0	-1.908495	0.002397	-0.112339
6	1	0	1.852045	-0.352761	0.815714
7	1	0	1.372922	-1.599976	-0.437671
8	1	0	1.146991	0.867913	-0.366874

TS3

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.273687	-0.312026	-0.047054
2	6	0	-0.006047	-0.749210	0.472767
3	6	0	1.132828	-0.017501	-0.048614
4	8	0	-2.241574	-0.740591	-0.545940
5	8	0	1.099437	1.105134	-0.530342
6	8	0	2.278850	-0.674501	0.077192
7	8	0	-1.270231	1.098719	0.522824
8	1	0	2.973246	-0.098889	-0.254256
9	1	0	-0.499029	0.447487	1.193860
10	1	0	0.136765	-1.801398	0.653869
11	1	0	-0.661405	1.615133	-0.045947

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.276885	-0.328755	-0.051239
2	6	0	0.001905	-0.745063	0.484806
3	6	0	1.145815	-0.008025	-0.056662
4	8	0	-2.240062	-0.760098	-0.568938
5	8	0	1.107931	1.105487	-0.568831
6	8	0	2.304778	-0.664706	0.100942
7	8	0	-1.310414	1.100477	0.554399
8	1	0	3.006148	-0.091633	-0.245367
9	1	0	-0.503445	0.456914	1.202510
10	1	0	0.151739	-1.800350	0.677569
11	1	0	-0.777319	1.676840	-0.036713

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.275175	-0.334896	-0.052223
2	6	0	0.003830	-0.741378	0.486615
3	6	0	1.144284	-0.003560	-0.060013
4	8	0	-2.228542	-0.761311	-0.572786
5	8	0	1.103723	1.097730	-0.579748
6	8	0	2.302636	-0.657141	0.108677
7	8	0	-1.315816	1.099081	0.561435
8	1	0	3.002078	-0.087804	-0.239178
9	1	0	-0.496773	0.454737	1.202157
10	1	0	0.158102	-1.794173	0.680444
11	1	0	-0.797042	1.679384	-0.030324

COCHCOOH (IM2)

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.475453	-0.250115	0.000177
2	6	0	-0.266063	-0.782723	0.000145
3	6	0	0.878518	0.104457	-0.000061
4	8	0	-2.532615	0.191145	0.000094
5	8	0	0.835176	1.308155	-0.000175
6	8	0	2.024501	-0.579505	-0.000115
7	1	0	2.735346	0.066326	-0.000257
8	1	0	-0.173850	-1.854395	0.000256

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.482246	-0.259059	0.000141
2	6	0	-0.266348	-0.797869	0.000117
3	6	0	0.880031	0.107470	-0.000085
4	8	0	-2.541133	0.195866	0.000184
5	8	0	0.827771	1.317311	-0.000243
6	8	0	2.041296	-0.576851	-0.000074
7	1	0	2.753936	0.080211	-0.000206
8	1	0	-0.166026	-1.874064	0.000234

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.481309	-0.257273	0.000152
2	6	0	-0.269406	-0.792219	0.000133
3	6	0	0.877610	0.111082	-0.000070
4	8	0	-2.531614	0.194850	0.000137
5	8	0	0.830281	1.313743	-0.000200
6	8	0	2.033672	-0.580142	-0.000100
7	1	0	2.748888	0.069524	-0.000239
8	1	0	-0.168973	-1.866677	0.000254

TS4

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.576488	-0.123283	0.005877
2	6	0	-0.319217	-0.447672	0.022878
3	6	0	0.835722	0.319386	-0.013861
4	8	0	-2.716327	0.051529	0.000360
5	8	0	1.316347	1.389960	0.002785
6	8	0	1.794753	-0.949935	-0.094033
7	1	0	2.466956	-0.994782	0.594015
8	1	0	0.734755	-1.428235	0.043725

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.582117	-0.135351	0.006773
2	6	0	-0.317755	-0.469579	0.026628
3	6	0	0.831530	0.325784	-0.013146
4	8	0	-2.726389	0.051020	-0.001465
5	8	0	1.299794	1.407718	0.002360
6	8	0	1.822432	-0.947170	-0.096863
7	1	0	2.496331	-0.980604	0.602314
8	1	0	0.747032	-1.437061	0.043899

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.579576	-0.137481	0.005000
2	6	0	-0.318327	-0.464106	0.015742
3	6	0	0.825997	0.333453	-0.014212
4	8	0	-2.714502	0.048354	0.003568
5	8	0	1.294725	1.405240	0.002785
6	8	0	1.821177	-0.950388	-0.092162
7	1	0	2.491028	-0.986555	0.605768
8	1	0	0.729206	-1.430290	0.041522

TS5

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.124171	-0.686073	0.071566
2	6	0	0.043901	-0.721810	0.818544
3	6	0	1.373591	0.078497	-0.089052
4	8	0	-1.931405	-1.052541	-0.646539
5	8	0	2.274391	-0.692933	-0.204930
6	8	0	1.081563	1.234059	-0.342249
7	8	0	-1.379250	1.332087	0.294729
8	1	0	-0.455475	1.578206	0.030475
9	1	0	-0.025223	-0.128473	1.719727
10	1	0	0.344727	-1.750426	0.974911
11	1	0	-1.986346	1.711629	-0.339553

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.159706	-0.653535	0.074579
2	6	0	-0.003028	-0.766689	0.840771
3	6	0	1.413685	0.081568	-0.100688
4	8	0	-1.959170	-1.000962	-0.679450
5	8	0	2.291549	-0.715342	-0.220077
6	8	0	1.106918	1.244171	-0.316472
7	8	0	-1.360808	1.318014	0.304633
8	1	0	-0.422948	1.564954	0.044867
9	1	0	-0.025907	-0.178025	1.752597
10	1	0	0.285156	-1.809230	0.953207
11	1	0	-1.969922	1.687186	-0.347713

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.163970	-0.627343	0.071305
2	6	0	0.005337	-0.770149	0.818195
3	6	0	1.401734	0.070558	-0.095112
4	8	0	-1.970789	-0.981196	-0.659819
5	8	0	2.282605	-0.712701	-0.228402
6	8	0	1.105780	1.235950	-0.300496
7	8	0	-1.341711	1.302953	0.299243
8	1	0	-0.395495	1.547945	0.054830
9	1	0	-0.009053	-0.206915	1.744777
10	1	0	0.272691	-1.818595	0.911233
11	1	0	-1.933818	1.679115	-0.361380

CH_3COOH

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.381664	-0.115474	-0.000003
2	6	0	0.088944	0.120526	-0.000011
3	8	0	0.630061	1.190799	0.000002
4	8	0	0.777951	-1.025323	-0.000003
5	1	0	1.711324	-0.797694	0.000033
6	1	0	-1.659430	-0.694777	0.875968
7	1	0	-1.659385	-0.695356	-0.875599
8	1	0	-1.900283	0.833712	-0.000310

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.392739	-0.119423	-0.000008
2	6	0	0.089543	0.123886	-0.000035
3	8	0	0.631727	1.200958	0.000005
4	8	0	0.785927	-1.032870	-0.000008
5	1	0	1.727452	-0.801188	0.000094
6	1	0	-1.667405	-0.701911	0.882484
7	1	0	-1.667284	-0.703616	-0.881398
8	1	0	-1.914822	0.835234	-0.000905

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.389730	-0.121726	0.000002
2	6	0	-0.090210	0.126761	-0.000002
3	8	0	-0.627247	1.198522	0.000000
4	8	0	-0.786285	-1.029484	-0.000004
5	1	0	-1.725085	-0.799147	0.000028
6	1	0	1.660161	-0.706056	-0.880557
7	1	0	1.660168	-0.705930	0.880640
8	1	0	1.915899	0.828621	-0.000074

C_3O_2

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.270310
3	6	0	0.000000	0.000000	-1.270310
4	8	0	0.000000	0.000000	2.424813
5	8	0	0.000000	0.000000	-2.424813

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.278521
3	6	0	0.000000	0.000000	-1.278521
4	8	0	0.000000	0.000000	2.439487
5	8	0	0.000000	0.000000	-2.439487

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.273743
3	6	0	0.000000	0.000000	-1.273743
4	8	0	0.000000	0.000000	2.425861
5	8	0	0.000000	0.000000	-2.425861

CH_2CO

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.204131
2	6	0	0.000000	0.000000	0.102278
3	8	0	0.000000	0.000000	1.259215
4	1	0	0.000000	0.936786	-1.731303
5	1	0	0.000000	-0.936786	-1.731303

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.211919
2	6	0	0.000000	0.000000	0.102870
3	8	0	0.000000	0.000000	1.266774
4	1	0	0.000000	0.942470	-1.739950
5	1	0	0.000000	-0.942470	-1.739950

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-1.205302
2	6	0	0.000000	0.000000	0.104208
3	8	0	0.000000	0.000000	1.258989
4	1	0	0.000000	0.940830	-1.732675
5	1	0	0.000000	-0.940830	-1.732675

CO_2

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.155402
3	8	0	0.000000	0.000000	-1.155402

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.162887
3	8	0	0.000000	0.000000	-1.162887

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	8	0	0.000000	0.000000	1.154909
3	8	0	0.000000	0.000000	-1.154909

H_2O

(i) MPWB1K/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.116613
2	1	0	0.000000	0.761601	-0.466450
3	1	0	0.000000	-0.761601	-0.466450

(ii) M06-2X/6-31+G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.115577
2	1	0	0.000000	0.768697	-0.462307
3	1	0	0.000000	-0.768697	-0.462307

(iii)M06-2X/6-311++G(d,p)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.116613
2	1	0	0.000000	0.761601	-0.466450
3	1	0	0.000000	-0.761601	-0.466450