Optimized B3LYP/aug-cc-pVTZ geometries, CCSD(T)/aug-cc-pVTZ energies

$CH_2OO + CH_4$ reaction

Isomer **1**(CH_3CH_2OOH)

Sum of electronic and zero-point Energies = -229.6563545

C	0.570931	0.629466	0.254338
O	-0.701201	0.576943	-0.387730
H	0.421586	0.715554	1.333560
H	0.977221	1.575663	-0.110207
O	-1.460747	-0.493710	0.241775
C	1.485273	-0.531862	-0.091336
H	1.071593	-1.474031	0.265685
H	1.638452	-0.598834	-1.169016
H	2.457954	-0.392104	0.383510
H	-1.608441	-1.077734	-0.513893

CH_2OO

Sum of electronic and zero-point Energies = -189.3004316

C	1.069800	-0.194558	0.000000
O	0.000000	0.459256	0.000000
H	1.030584	-1.277037	0.000000
H	1.974124	0.396906	0.000000
O	-1.177938	-0.203321	0.000000

CH_3CH_2O

Sum of electronic and zero-point Energies = -154.0679688

C	0.179025	0.474895	-0.000190
O	1.255779	-0.362933	-0.000232
C	-1.188099	-0.194666	-0.000007
H	0.300783	1.159260	-0.861263
H	0.302065	1.154843	0.864488
H	-1.306282	-0.820839	-0.884268
H	-1.304715	-0.823904	0.882267
H	-1.983639	0.552730	0.001813

TS1

Sum of electronic and zero-point Energies = -229.6563545

C	-0.168127	1.013835	0.230017
O	-1.032663	0.258066	-0.364981
H	-0.040701	0.920979	1.300125
H	0.002691	1.966982	-0.258529
O	-0.861604	-1.027519	0.178009
C	1.620422	-0.229050	-0.095722
H	2.141125	-0.934781	0.559641
H	1.800677	-0.463812	-1.143780
H	2.069973	0.740797	0.112817
H	0.466601	-0.783250	0.119724

TS2

Sum of electronic and zero-point Energies = -229.6957815

C		-0.465075	0.269269	0.453251
O		0.375503	0.904927	-0.318663
C		-1.656517	-0.426056	-0.187835
H		-0.633073	0.753453	1.428923
H		-2.385729	0.314088	-0.522282
H		-2.142884	-1.087368	0.529028
H		-1.336129	-1.008605	-1.050132
H		0.355357	-0.597783	0.756199
O		1.661461	-0.491489	0.006561
1	0	2.576306	-0.740561	-0.237420

TS3

Sum of electronic and zero-point Energies = -229.6813895

C	0.918232	-0.418928	0.271696
O	-0.034700	-1.154576	-0.252138
C	0.814314	1.042425	-0.136878
H	1.863134	-0.654591	-0.294182
H	1.097625	-0.546385	1.347784
H	0.867297	1.227869	-1.207579
H	1.422164	1.734046	0.440269
H	-0.389136	0.989946	0.080157
O	-1.646154	0.409011	0.111846
H	-1.809526	-0.527347	-0.053024

TS5

Sum of electronic and zero-point Energies = -229.6534207

C	0.448808	-1.044912	-0.056001
O	1.339631	-0.169661	0.064503
C	-1.575168	-0.254245	0.031620
H	0.181131	-1.639000	0.825531
H	0.258360	-1.477833	-1.045330
H	-1.712970	0.058548	1.052006
H	-1.776409	-1.292205	-0.185908
H	-1.892255	0.436718	-0.728526
O	0.094856	1.344099	-0.035383
H	0.224406	2.313204	-0.004446

TS6

Sum of electronic and zero-point Energies = -154.0395105

C	-0.574585	0.547662	0.000000
O	-1.243117	-0.481528	0.000000
C	1.521983	-0.164316	0.000000
H	-0.379687	1.103571	0.932385
H	-0.379687	1.103570	-0.932386
H	2.025538	0.792075	0.000032
H	1.497177	-0.723559	0.922431
H	1.497200	-0.723509	-0.922462

TS7

Sum of electronic and zero-point Energies = -154.0327304

C	-0.223426	0.300104	-0.221503
O	-1.217461	-0.341416	0.076725
C	1.185526	-0.165858	0.046700
H	-0.323744	1.622039	1.069093
H	-0.316276	1.176313	-0.895197
H	1.540742	-0.685124	-0.848782
H	1.857130	0.673166	0.226506
H	1.209237	-0.860538	0.883397

$CH_3CHOO + CH_4$ reaction

Isomer **1**$(CH_3)_2CHOOH$

Sum of electronic and zero-point Energies = -268.989704

C	0.524838	0.012689	0.459112
O	-0.883543	-0.062262	0.742430
C	1.021217	-1.232732	-0.261515
H	0.918669	0.022043	1.480181
H	0.725109	-2.130548	0.279864
H	2.109503	-1.215608	-0.334235
H	0.612122	-1.285081	-1.269554
O	-1.612228	-0.131859	-0.517585
C	0.903303	1.312383	-0.237971
H	0.508857	1.338836	-1.253334
H	0.519232	2.171661	0.312461
H	1.988562	1.403861	-0.296758
H	-2.112032	0.693763	-0.475146

syn-CH_3CHOO

Sum of electronic and zero-point Energies = -228.5320864

C	0.481784	0.697590	-0.000048
O	-0.774843	0.588580	0.000027
H	0.816840	1.727863	-0.000090
C	1.364337	-0.472685	-0.000073
H	1.129970	-1.098354	-0.867006
H	1.130197	-1.098223	0.867017
H	2.410539	-0.180727	-0.000221
O	-1.295691	-0.676079	0.000102

anti-CH_3CHOO

Sum of electronic and zero-point Energies = -228.5265338

C	-0.380511	0.407665	0.000055
O	0.571544	-0.409438	-0.000103
H	-0.120046	1.462482	0.000216
C	-1.768542	-0.097931	0.000050
H	-1.787220	-1.185029	-0.000627
H	-2.303647	0.276214	-0.876934
H	-2.303224	0.275062	0.877794
O	1.854513	0.073546	-0.000032

$(CH_3)_2CHO$

Sum of electronic and zero-point Energies = -193.2857443

C	0.022639	0.126313	0.365000
O	-0.226425	1.368849	-0.156661
C	1.354554	-0.460169	-0.100741
C	-1.184645	-0.740517	-0.093173
H	-0.020369	0.165235	1.464998
H	1.366044	-0.568180	-1.185698
H	1.522925	-1.438231	0.353603
H	2.176010	0.195173	0.187846
H	-2.119694	-0.317264	0.266058
H	-1.210261	-0.800263	-1.179877
H	-1.058540	-1.741022	0.319843

TS1

Sum of electronic and zero-point Energies = -268.8839027

C	-0.512201	-0.210085	0.380551
O	0.210222	-1.048017	-0.302690
C	-1.908925	0.000020	-0.076661
O	1.548852	-0.828902	0.080577
H	-0.257021	-0.086120	1.425178
H	-1.992202	-0.122598	-1.154117
H	-2.240713	0.999443	0.202465
H	-2.573797	-0.714101	0.417163
C	0.692105	1.624442	-0.088593
H	1.668401	2.096749	0.078172
H	0.400373	1.782645	-1.124717
H	-0.001183	2.135435	0.575479
H	1.297676	0.437637	0.065505

TS2

Sum of electronic and zero-point Energies = -268.8793495

C	0.557038	0.083259	0.620855
O	0.008102	-1.099821	0.583197
C	1.476245	0.594346	-0.438543
H	0.763493	0.378227	1.647618
H	2.471753	0.181611	-0.241684
H	1.553322	1.678739	-0.386427
H	1.156093	0.289692	-1.428358
O	-0.642849	-1.223205	-0.661439
C	-1.271428	1.218745	0.028281
H	-1.387487	1.736382	-0.926897
H	-2.240790	1.002264	0.479740
H	-0.765048	1.916457	0.693071
H	-1.044492	0.022733	-0.474685

TS3

Sum of electronic and zero-point Energies = -268.9129397

C	0.351430	0.001885	0.005964
O	-0.593505	-0.021718	0.930262
C	1.163537	-1.285050	-0.159353
C	1.097616	1.332887	-0.150863
H	-0.571007	-0.006221	-0.856533
H	1.912111	-1.370231	0.639691
H	1.691908	-1.297862	-1.118410
H	0.502632	-2.154331	-0.104622
H	0.396286	2.170579	-0.094943
H	1.836598	1.451562	0.652312
H	1.629050	1.376444	-1.107133
O	-1.977736	-0.124747	-0.402705
H	-2.503147	0.703441	-0.405316

TS5

Sum of electronic and zero-point Energies = -268.880257

C	-0.689868	-0.093839	0.525828
O	-0.059630	-1.163308	0.668916
C	-1.651518	0.101858	-0.620059
H	-0.830942	0.501419	1.438757
H	-2.001962	1.130919	-0.695592
H	-2.521284	-0.541535	-0.464982
H	-1.173842	-0.193939	-1.552338
C	0.780493	1.580579	0.179880
H	1.408349	1.441072	1.043425
H	-0.103918	2.187884	0.286804
H	1.269124	1.616584	-0.775741
O	1.453958	-0.647641	-0.527845
H	2.165212	-1.186400	-0.922791

TS6

Sum of electronic and zero-point Energies = -268.8987442

C	0.472815	-0.085598	0.398650
O	-0.174275	-1.083852	-0.164393
C	-0.030468	1.254456	-0.096001
C	2.000697	-0.155917	-0.108802
H	0.499631	-0.115422	1.499534
H	0.037919	1.401023	-1.172503
H	0.306896	2.122455	0.464874
H	2.550802	0.676016	0.320548
H	2.027905	-0.124622	-1.193534
H	2.397232	-1.100179	0.251272
H	-1.182297	0.879460	0.054509
O	-2.230105	-0.022238	0.002908
H	-2.061310	-0.967659	-0.095901

TS7

Sum of electronic and zero-point Energies = -193.2621824

C	-0.311446	0.274535	0.382655
O	-0.290070	1.366950	-0.198456
C	1.658516	-0.438153	-0.079090
C	-1.167199	-0.875173	-0.108214
H	-0.032221	0.226551	1.452015
H	1.559630	-0.535647	-1.149909
H	1.682733	-1.349181	0.502360
H	2.242592	0.395034	0.280353
H	-2.194334	-0.686735	0.216635
H	-1.162440	-0.921768	-1.195957
H	-0.854618	-1.831114	0.310048

TS8

Sum of electronic and zero-point Energies = -193.2550899

C	-0.000001	0.169901	0.042691
O	-0.000003	1.390367	-0.109634
C	1.294181	-0.623819	-0.049987
C	-1.294178	-0.623823	-0.049987
H	0.000000	0.261016	1.826488
H	1.405805	-0.957423	-1.085964
H	1.284275	-1.510489	0.581982
H	2.141182	0.009170	0.201122
H	-2.141182	0.009163	0.201119
H	-1.405800	-0.957431	-1.085964
H	-1.284270	-1.510491	0.581984

$(CH_3)_2COO + CH_4$ reaction

Isomer **1**$(CH_3)_3COOH$

Sum of electronic and zero-point Energies = -308.2118403

C	-0.388992	-0.000056	0.034739
O	0.738328	0.064727	-0.876992
C	-1.568412	0.138744	-0.927236
C	-0.409766	-1.351556	0.745815
H	-1.529207	1.091565	-1.454622
H	-2.504049	0.090364	-0.370352
H	-1.561192	-0.665577	-1.661889
H	-0.426426	-2.162993	0.018414
H	-1.296552	-1.432789	1.375658
H	0.469735	-1.470685	1.375646
O	1.978781	-0.098653	-0.135031
C	-0.343306	1.162431	1.025053
H	0.524391	1.083629	1.678265
H	-0.300394	2.115251	0.495803
H	-1.236205	1.160300	1.651105
H	2.385885	0.764968	-0.282073

$(CH_3)_2COO$

Sum of electronic and zero-point Energies = -267.7587605

C	0.378055	0.024809	-0.000028
O	-0.567029	-0.816222	-0.000049
C	1.751770	-0.540879	0.000016
C	0.071752	1.465329	-0.000026
O	-1.857668	-0.326479	0.000034
H	1.722556	-1.627513	-0.000319
H	2.301624	-0.192337	0.877845
H	2.301998	-0.191799	-0.877357
H	-0.557287	1.694495	-0.864785
H	0.975459	2.068708	-0.000564
H	-0.556239	1.694507	0.865526

$(CH_3)_3CO$

Sum of electronic and zero-point Energies = -232.506446

C	0.000051	-0.027832	0.082332
O	-0.000308	0.268915	1.426665
C	-1.272663	-0.794109	-0.311702
C	-0.002068	1.383969	-0.582035
C	1.274946	-0.790402	-0.311808
H	-1.300446	-0.979025	-1.386406
H	-2.158439	-0.227501	-0.027661
H	-1.301955	-1.755964	0.200653
H	-0.001575	1.245120	-1.663455
H	0.884232	1.943915	-0.291483
H	-0.890303	1.941057	-0.291909
H	2.159134	-0.220907	-0.028581
H	1.302786	-0.975966	-1.386399
H	1.307434	-1.751804	0.201199

TS1

Sum of electronic and zero-point Energies = -308.1068796

C	-0.495322	-0.169860	-0.013966
O	0.302361	-0.850699	-0.804827
C	-1.735994	0.297231	-0.703656
C	-0.569852	-0.484078	1.449864
H	-1.562035	0.433505	-1.767866
H	-2.070878	1.238025	-0.268285
H	-2.539151	-0.431173	-0.561550
H	-1.259523	-1.326633	1.574494
H	-0.972591	0.358676	2.007031
H	0.398941	-0.761909	1.847328
O	1.594446	-0.846373	-0.242580
C	0.904617	1.630940	0.116191
H	1.784749	1.948300	0.687382
H	0.963661	2.029427	-0.895495
H	0.048355	2.066053	0.624538
H	1.413325	0.376902	0.041084

TS2

Sum of electronic and zero-point Energies = -308.1212374

C	-0.404511	0.063056	-0.044276
O	0.286622	-0.132746	-1.146623
C	0.173884	-0.774594	1.092936
C	-1.837160	-0.673696	-0.299774
C	-0.625459	1.530221	0.330535
H	0.225311	-1.842106	0.890711
H	-0.217205	-0.562609	2.084780
H	1.292549	-0.397498	0.816428
H	-2.426002	-0.623478	0.610242
H	-1.674241	-1.700339	-0.608260
H	-2.313117	-0.109928	-1.096248
H	-1.254085	1.640879	1.214685
H	-1.090030	2.057024	-0.502037
H	0.343626	1.987834	0.526282
O	2.347716	-0.034690	-0.032017
H	2.197970	0.019789	-0.983988

TS4

Sum of electronic and zero-point Energies = -308.0957093

C	0.521881	-0.251703	-0.115948
O	-0.252846	-0.940974	-0.847417
C	0.948386	-0.843323	1.216471
C	1.520561	0.626924	-0.858990
H	1.438195	-0.115575	1.863602
H	1.659175	-1.653083	1.030010
H	0.083941	-1.261785	1.727095
H	1.935062	1.411120	-0.224223
H	1.056479	1.071282	-1.736449
H	2.350062	-0.000573	-1.194626
H	-0.674932	1.485416	0.610818
H	-0.781374	2.000759	-0.328394
H	0.241266	1.629415	1.161244
H	-1.560782	1.418689	1.216795
O	-1.933724	-0.304760	-0.180127
H	-2.824837	-0.638258	-0.408809

TS5

Sum of electronic and zero-point Energies = -232.4835988

C	-0.287629	0.000000	0.207487
O	-0.102265	0.000001	1.441764
C	-0.723391	1.292064	-0.478844
C	1.754385	0.000001	-0.342840
C	-0.723389	-1.292067	-0.478842
H	-0.529664	1.290311	-1.550348
H	-0.240859	2.148842	-0.014345
H	-1.802714	1.393893	-0.335085
H	1.673393	0.000017	-1.421000
H	2.085663	-0.916040	0.122325
H	2.085672	0.916026	0.122351
H	-0.240873	-2.148843	-0.014325
H	-0.529638	-1.290325	-1.550342
H	-1.802715	-1.393885	-0.335106

Dissociation fragments

OH

Sum of electronic and zero-point Energies = -75.6371645

O	0.000000	0.000000	0.108368
H	0.000000	0.000000	-0.866946

CO

Sum of electronic and zero-point Energies = -113.1569402

C	0.000000	0.000000	-0.643325
O	0.000000	0.000000	0.482493

CH_3

Sum of electronic and zero-point Energies = -39.7339644

C	0.000052	0.000049	-0.000
H	-0.739074	0.784747	0.000
H	1.049289	0.247247	0.000
H	-0.310526	-1.032289	0.000

CH_4

Sum of electronic and zero-point Energies = -40.3963823

C	0.000022	-0.000005	-0.000198
H	0.620930	-0.873173	-0.190716
H	-0.347590	-0.020451	1.031059
H	0.583279	0.903254	-0.168149
H	-0.856752	-0.009597	-0.671005

H_2O

Sum of electronic and zero-point Energies = -76.3210605

O	0.000000	0.116984	0.000000
H	0.763385	-0.467935	0.000000
H	-0.763385	-0.467935	0.000000

Acetone $(CH_3)_2CO$

Sum of electronic and zero-point Energies = -192.7685449

C	0.000004	0.184293	-0.000007
O	-0.000026	1.394552	0.000000
C	-1.287712	-0.611460	0.001257
C	1.287740	-0.611435	-0.001268
H	-1.301308	-1.316831	0.834639
H	-1.359290	-1.203203	-0.914333
H	-2.141223	0.057566	0.068662
H	2.141224	0.057587	-0.069004
H	1.359439	-1.202830	0.914540
H	1.301180	-1.317096	-0.834396

Methanol CH_3OH

Sum of electronic and zero-point Energies = -115.5113068

C	-0.667417	0.020463	-0.000001
O	0.748803	-0.122100	-0.000001
H	-1.026809	0.543754	0.891054
H	-1.083678	-0.984792	-0.000570
H	-1.026717	0.544753	-0.890498
H	1.151281	0.750305	0.000033

2-Butanone $CH_3CH_2COCH_3$

Sum of electronic and zero-point Energies = -231.9808719

C	-0.563138	0.219712	0.101155
O	-0.959989	1.323392	-0.200588
C	0.824814	0.014990	0.684998
C	1.861557	-0.203469	-0.428454
C	-1.413621	-1.014656	-0.104236
H	1.079575	0.907954	1.255147
H	0.825096	-0.841383	1.362562
H	2.855822	-0.333853	-0.001936
H	1.888885	0.654347	-1.099604
H	1.635343	-1.091352	-1.020560
H	-0.842656	-1.808552	-0.589177
H	-2.294850	-0.773533	-0.692645
H	-1.724982	-1.400223	0.870136

Formaldehyde CH_2O

Sum of electronic and zero-point Energies = -114.3162554

C	0.000000	0.000000	-0.526996
O	0.000000	0.000000	0.673449
H	0.000000	0.937799	-1.112807
H	0.000000	-0.937799	-1.112807

Acetaldehyde CH_3CHO

Sum of electronic and zero-point Energies = -153.5431118

C	-0.232392	0.396229	0.000125
O	-1.232033	-0.275785	-0.000031
C	1.165419	-0.148490	-0.000056
H	-0.306421	1.503721	-0.000158
H	1.701020	0.224439	0.876949
H	1.701826	0.227538	-0.875222
H	1.161671	-1.235846	-0.001737

Propaldehyde CH_3CH_2CHO

Sum of electronic and zero-point Energies = -192.7560005

C	-0.783436	-0.222715	0.306886
O	-1.809324	-0.046848	-0.299448
C	0.471591	0.592090	0.143655
C	1.686309	-0.287557	-0.176204
H	-0.710792	-1.043975	1.052811
H	0.303261	1.345663	-0.624974
H	0.641842	1.110675	1.093921
H	2.594829	0.312211	-0.211969
H	1.570327	-0.780587	-1.141593
H	1.828351	-1.060109	0.581358

H atom

Sum of electronic and zero-point Energies = -0.4998212