A Theoretical Study of the Reaction of CH_3 with HOCO Radicals

Supplementary Table

Hua-Gen Yu

Department of Chemistry

Brookhaven National Laboratory

Upton, New York 11973-5000

Joseph S. Francisco*

Department of Chemistry

Purdue University

West Lafayette, Indiana 47907-2084

The CCSD(T)/avdz Optimized Coordinates (Angstroms) of the stationary points for the CH3 + HOCO reaction

Structure of CH2COOH

H	-1.757870	-0.616152	0.001155
O	-0.854906	-0.976849	-0.000372
C	-0.018969	0.113010	-0.000224
O	-0.436363	1.267701	0.000287
C	1.394982	-0.266647	0.000019
H	2.141704	0.530303	-0.002126
H	1.690238	-1.319153	0.002878

8

Structure of the TS to CH4 + CO2 via a direct H-abstraction optimized at mp2/atdz

O	0.662773	-1.294452	-0.082993
C	0.885047	-0.147961	0.025407
O	1.134997	1.013981	0.114602
H	0.253467	2.345845	-0.816529
C	-2.273662	0.070807	0.060022
H	-2.461775	1.075638	-0.331164
H	-1.798539	0.003197	1.045639
H	-2.043621	-0.717984	-0.663382

Structure for acetic acid optimized at CCSD(T)/avdz

C	1.404222	-0.117209	-0.00001
C	-0.090035	0.127946	0.000007
O	-0.641950	1.215245	0.000011
H	1.930679	0.847809	-0.001322
O	-0.788829	-1.052215	0.000028
H	-1.729975	-0.804887	-0.000184
H	1.680485	-0.704684	0.892743
H	1.679924	-0.706907	-0.891474

Structure for enediol optimized at CCSD(T)/avdz

C	-0.077138	-0.031940	0.000066
C	-1.419346	-0.200318	0.000055
O	0.602157	1.167234	-0.000127
H	-2.087224	0.664474	-0.000624
H	-1.836877	-1.208497	0.000515
O	0.804237	-1.073676	-0.000198
H	1.697013	-0.697351	0.001215
H	-0.045158	1.886451	0.000768

Structure for ch3c(o)oh → ch2=c=o + h2o transition state optimized at CCSD(T)/avdz

C	-0.270986	1.322044	-0.058107
C	0.460782	0.090696	0.002672
H	-1.243481	0.364966	-0.412159
O	-1.194880	-0.797887	0.084629
O	1.421206	-0.579901	0.025969
H	-1.227982	-1.488119	-0.599181
H	-0.776278	1.491861	0.905835
H	0.298352	2.177157	-0.446669

Structure for ch3c(o)oh → ch4+ co2 transition state optimized at CCSD(T)/avdz

C	-0.416767	-0.010712	-0.000002
O	-0.538053	1.262925	0.000009
H	0.718422	0.896360	-0.000100
C	1.475371	-0.253090	0.000034
O	-1.026220	-1.033003	-0.000007
H	2.257027	0.546143	-0.001113
H	1.593195	-0.850320	-0.915781
H	1.593915	-0.848740	0.916783

Structure for ch2c(oh)2 -→ ch2=c=o + h2o transition state optimized at CCSD(T)/avdz

C	-0.213011	0.182195	-0.012573
O	0.920682	-0.934964	-0.101195
O	0.580739	1.195529	0.017506
H	1.418367	0.121899	-0.009356
H	0.949879	-1.417567	0.744993
C	-1.507597	-0.200407	0.003925
H	-1.780041	-1.252091	-0.087411
H	-2.275922	0.572508	0.073173

Structure for ch3c(o)oh → ch2c(oh)2 transition state optimized at CCSD(T)/avdz

C	0.050914	-0.030475	0.034123
C	-1.256078	-0.612625	-0.053753
O	-0.015421	1.271412	-0.008622
H	-1.168894	0.887382	-0.364785
O	1.230319	-0.651185	0.034059
H	1.917487	0.021326	-0.118561
H	-1.377824	-1.632145	-0.439989
H	-1.858973	-0.379779	0.837617

Structure for ch2=c=o optimized at CCSD(T)/avdz

C	.000000	.000000	-1.231348
C	.000000	.000000	.105767
O	.000000	.000000	1.284409
H	.000000	.953958	-1.760892
H	.000000	-.953958	-1.760892

Structure for ch3co optimized at CCSD(T)/avdz

C	-.981513	-.666178	.000000
C	.000000	.507033	.000000
O	1.197097	.467802	.000000
H	-.438069	-1.629004	.000000
H	-1.624814	-.579269	.892426
H	-1.624814	-.579269	-.892426

Structure for formic acid optimized at CCSD(T)/avdz

C	.000000	.426595	.000000
O	1.173032	.111995	.000000
O	-1.043496	-.447413	.000000
H	-.654912	-1.341099	.000000
H	-.381374	1.464880	.000000