

Electronic supplementary information for

**Multi-path Variational Transition State Theory for Chemical Reaction  
Rates of Complex Polyatomic Species: Ethanol + OH Reactions**

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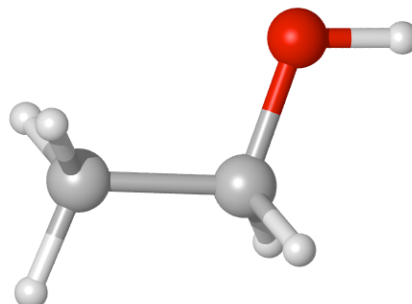
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Cartesian coordinates optimized by the M08-HX/6-31+G(d,p) method (in Å). Only one structure of each pair of mirror images is listed.

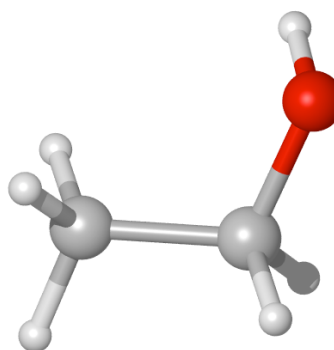
Ethanol (trans)

C	1.219082	-0.221696	0.000000
H	1.281446	-0.862427	-0.888538
H	1.281446	-0.862427	0.888538
H	2.077249	0.462513	0.000001
C	-0.086449	0.550118	0.000000
H	-0.144817	1.199152	0.891691
H	-0.144816	1.199152	-0.891691
O	-1.144613	-0.395998	0.000000
H	-1.989396	0.061481	-0.000002



Ethanol (gauche)

C	-1.210872	-0.239559	-0.021067
H	-1.275068	-0.961827	0.806071
H	-1.268132	-0.796268	-0.965000
H	-2.084238	0.422744	0.048137
C	0.084667	0.557786	0.046769
H	0.131092	1.284849	-0.774656
H	0.137400	1.128733	0.990682
O	1.232759	-0.259788	-0.107595
H	1.254108	-0.909293	0.601309

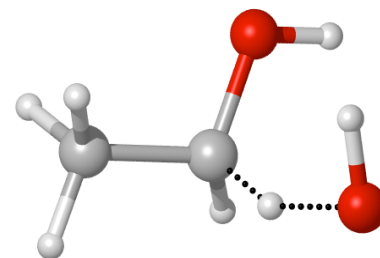


OH radical

O	0.000000	0.000000	0.108294
H	0.000000	0.000000	-0.866350

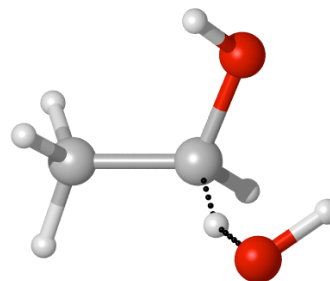
Reaction R1a TS 1, 2

C	1.347593	-0.904637	-0.181662
H	2.374335	-0.514956	-0.183595
H	1.044905	-1.076384	-1.222242
H	1.333755	-1.864050	0.348860
C	0.415819	0.083359	0.480090
H	-0.655765	-0.359826	0.501537
H	0.671368	0.260905	1.539074
O	0.400505	1.274020	-0.262998
H	-0.077715	1.954274	0.220590
O	-2.075434	-0.454068	-0.004116
H	-1.871915	-0.031917	-0.857874



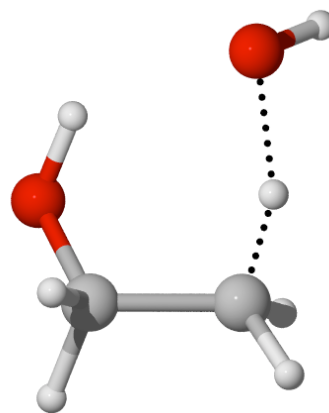
Reaction R1a TS 3, 4

C	1.414994	-0.861109	-0.175119
H	1.420000	-1.839647	0.320300
H	2.421300	-0.425898	-0.104977
H	1.178639	-1.025262	-1.236092
C	0.397651	0.061760	0.468436
H	-0.642882	-0.437018	0.371471
H	0.569954	0.200770	1.543927
O	0.346478	1.340492	-0.102400
H	0.304840	1.255574	-1.061034
O	-2.078997	-0.510029	-0.108421
H	-2.267560	0.423876	0.093061



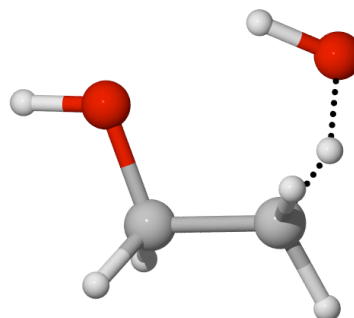
Reaction R1b TS 1, 2

C	0.140544	1.187626	-0.215972
H	-0.930212	0.760515	0.034869
H	0.190594	2.164507	0.280668
H	0.193351	1.285000	-1.306759
C	1.109199	0.155664	0.327887
H	2.144207	0.448668	0.094924
H	1.023808	0.101027	1.427585
O	0.904584	-1.108499	-0.262352
H	-0.009305	-1.364522	-0.079699
O	-1.877181	-0.296738	0.203630
H	-2.330129	-0.213040	-0.653304



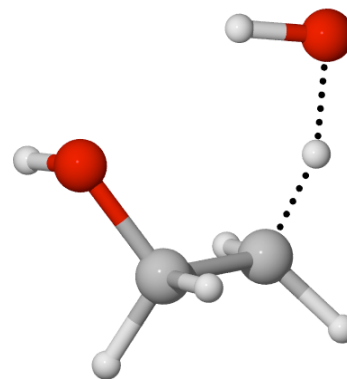
Reaction R1b TS 3, 4

C	0.007272	1.188995	-0.228741
H	1.074081	0.650226	-0.051752
H	-0.079968	1.311012	-1.313877
H	0.073448	2.152591	0.287498
C	-1.037538	0.267267	0.347082
H	-0.907613	0.180104	1.438759
H	-2.049687	0.663863	0.150739
O	-0.871725	-1.001877	-0.277772
H	-1.524549	-1.622025	0.058228
O	1.911311	-0.372542	0.130676
H	1.279196	-1.077987	-0.102882



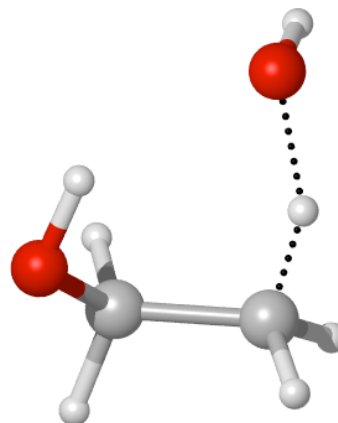
Reaction R1b TS 5, 6

C	-0.018063	1.189903	0.238877
H	1.061299	0.660454	0.092023
H	0.050691	2.155457	-0.275030
H	-0.127490	1.325167	1.322356
C	-1.032784	0.244734	-0.367644
H	-2.061802	0.612501	-0.209462
H	-0.876866	0.161798	-1.451009
O	-0.890933	-1.077849	0.139123
H	-1.171919	-1.103108	1.059055
O	1.912302	-0.341343	-0.101991
H	1.260220	-1.066556	-0.062387



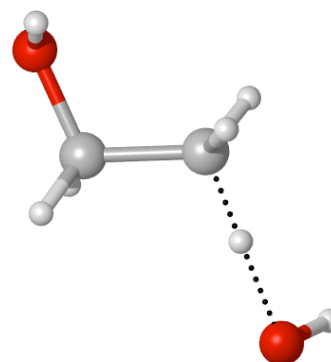
Reaction R1b TS 7, 8

C	-0.126207	1.186674	-0.250362
H	0.949306	0.703233	-0.250223
H	-0.333047	1.338818	-1.316871
H	-0.057917	2.139743	0.287869
C	-1.050309	0.170202	0.390756
H	-0.825236	0.079430	1.469627
H	-2.096383	0.501548	0.307298
O	-0.970517	-1.081377	-0.251426
H	-0.043897	-1.355745	-0.238664
O	1.880021	-0.354849	0.004095
H	2.190236	-0.058476	0.877246



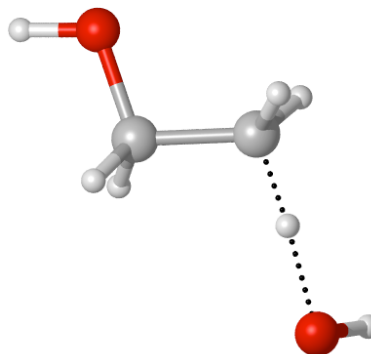
Reaction R1b TS 9, 10

C	0.160922	0.701497	0.017397
H	1.261912	0.278169	0.130207
H	0.105668	1.254456	-0.927675
H	0.045443	1.386297	0.868222
C	-0.791732	-0.479691	0.050462
H	-0.569840	-1.172153	-0.771024
H	-0.680573	-1.040357	0.992974
O	-2.135728	-0.067114	-0.144209
H	-2.422232	0.451504	0.613436
O	2.539137	-0.254921	0.078560
H	2.817208	0.087530	-0.788102



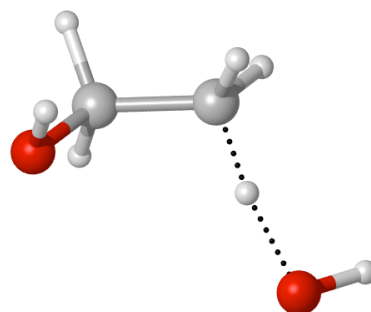
Reaction R1b TS 11, 12

C	-0.165998	0.732852	0.056629
H	-1.269720	0.303541	0.154444
H	-0.029904	1.375944	0.933633
H	-0.114963	1.319046	-0.868050
C	0.768663	-0.455533	0.042121
H	0.647114	-1.039788	0.969539
H	0.525223	-1.115238	-0.807957
O	2.090117	0.053226	-0.070897
H	2.718225	-0.674251	-0.054546
O	-2.500636	-0.298017	0.051934
H	-2.807810	0.125164	-0.767860



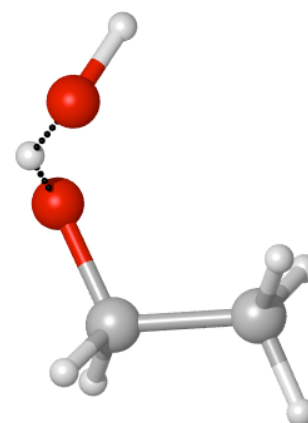
Reaction R1b TS 13, 14

C	-0.149899	0.912636	0.297586
H	-1.036783	0.136131	0.147875
H	-0.026116	0.999203	1.385898
H	-0.479748	1.872247	-0.119316
C	1.074870	0.365631	-0.407325
H	0.859262	0.192214	-1.469700
H	1.886200	1.118267	-0.359008
O	1.508012	-0.875291	0.106350
H	1.682726	-0.790627	1.048354
O	-2.209081	-0.549164	-0.084281
H	-2.826815	0.198601	-0.152216



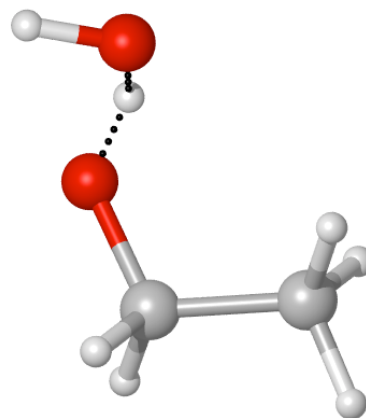
Reaction R1c TS 1, 2

C	-1.383929	0.810831	-0.142210
H	-1.624204	0.749728	-1.211062
H	-0.628169	1.593337	0.006738
H	-2.292024	1.092428	0.406663
C	-0.844511	-0.521426	0.357169
H	-0.594828	-0.477165	1.429495
H	-1.599497	-1.315816	0.221908
O	0.266329	-0.959952	-0.389779
H	1.180138	-0.556604	0.025872
O	1.842953	0.503905	0.204265
H	2.054968	0.826039	-0.685249



Reaction R1c TS 3, 4

C	-1.381637	-0.802206	-0.133682
H	-0.626146	-1.588625	-0.003172
H	-1.643509	-0.740544	-1.197658
H	-2.278791	-1.091711	0.428551
C	-0.845014	0.528977	0.364457
H	-1.588809	1.335517	0.245404
H	-0.598957	0.485675	1.439539
O	0.276896	0.977506	-0.360227
H	0.976003	0.168387	-0.508648
O	1.808402	-0.594487	0.073970
H	2.437726	0.006523	0.501385



Reaction R1c TS 5, 6

C	2.043550	-0.033487	0.011320
H	2.251736	-0.612076	-0.896555
H	2.226014	-0.674405	0.882311
H	2.733602	0.818941	0.051352
C	0.603004	0.468435	0.011253
H	0.407280	1.055387	0.923588
H	0.407441	1.109684	-0.862533
O	-0.230550	-0.669676	-0.013146
H	-1.230484	-0.404831	-0.355190
O	-2.280342	0.205988	-0.066820
H	-2.587776	-0.192880	0.761323

