

Solvent-Dependent Transition States For Decarboxylations

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The supporting information is given below. It consists of 9 Gaussian input files, each defining, in Cartesian coordinates, an optimized stationary point reported in the manuscript. Structure names identify the chemical form:

- a - acidic form
  - z - zwitterionic form
  - ts - transition state
- and the phase:
- gas - gas phase
  - aq - aqueous solution
  - d - dioxane solution

This information is explicitly repeated in the comment line in each case.

Energies of these species are also listed in the comment line (HF energies for the gas phase results and Gs(liq) for results obtained with SM5.42).

1\*\*\*\*\* a-aq \*\*\*\*\*

%SUBST I502 /home/smpa/paneth/SMx  
 %SUBST I701 /home/smpa/paneth/SMx  
 %SUBST I716 /home/smpa/paneth/SMx  
 # rhf/6-31g(d) iop(5/40=3000)

acid, water, Gs(liq): -473.365346966

0	1					
C						
C	1	1.382086				
N	2	1.324444	1	123.896018		
C	3	1.323777	2	116.967412	1	-0.010847
C	4	1.382253	3	123.849714	2	0.013548
C	1	1.386775	2	118.880909	3	0.046058
C	6	1.516506	1	121.587120	2	-179.667571
C	7	1.509564	6	110.967008	1	91.013213
O	8	1.197931	7	124.532089	6	101.631027
O	8	1.324246	7	112.328124	6	-77.835922
H	1	1.074371	2	119.998435	3	-179.887887
H	2	1.074919	1	119.955048	6	-179.824936
H	4	1.074936	3	116.205525	2	-179.864338
H	5	1.074566	4	119.967516	3	-179.919889
H	7	1.080089	6	110.462371	1	-149.798209
H	7	1.082425	6	110.051910	1	-29.372531
H	10	0.959014	8	109.994200	7	178.739804

2\*\*\*\*\* a-d \*\*\*\*\*

%SUBST 1502 /home/paneth  
 %SUBST 1701 /home/paneth  
 %SUBST 1716 /home/paneth  
 # rhf/6-31g(d) iop(5/40=3000)

acid, dioxan, Gs(liq) -473.359901967

0 1

C						
C	1	1.384078				
N	2	1.320730	1	123.724533		
C	3	1.321967	2	117.337580	1	0.041336
C	4	1.382659	3	123.699438	2	-0.094568
C	1	1.385809	2	118.829250	3	0.110847
C	6	1.516908	1	121.660997	2	-179.706269
C	7	1.510064	6	110.881856	1	99.864657
O	8	1.192039	7	124.724970	6	100.794653
O	8	1.326060	7	112.291939	6	-78.439776
H	1	1.074443	2	120.049746	3	-179.848803
H	2	1.075554	1	120.029517	6	-179.811047
H	4	1.075465	3	116.243248	2	-179.968329
H	5	1.074726	4	120.147997	3	179.956337
H	7	1.080785	6	110.400131	1	-141.218681
H	7	1.082259	6	110.166549	1	-20.752083
H	10	0.955919	8	109.212753	7	178.175829

3\*\*\*\*\* a-gas \*\*\*\*\*

# rhf/6-31g(d)

acid, gas phase: -473.3476572

0 1

C	-1.200993	0.317739	-1.070630		
C	-1.015217	-0.173467	-2.352941		
N	0.166258	-0.466835	-2.860949		
C	1.222972	-0.277284	-2.089986		
C	1.153223	0.209237	-0.797192		
C	-0.091596	0.519725	-0.266557		
C	-0.219151	1.053245	1.147988		
C	0.054644	-0.037361	2.158156		
O	1.092354	-0.208988	2.708146		
O	-1.003259	-0.815999	2.355085		
H	-2.191713	0.534311	-0.715226		
H	-1.862967	-0.335390	-2.995444		
H	2.176704	-0.523419	-2.522583		
H	2.049052	0.338941	-0.217651		
H	0.503708	1.839416	1.318852		
H	-1.214105	1.446196	1.311296		
H	-0.760543	-1.503323	2.968515		

4\*\*\*\*\* ts-aq \*\*\*\*\*

%SUBST I502 /home/smpa/paneth/SMx  
 %SUBST I701 /home/smpa/paneth/SMx  
 %SUBST I716 /home/smpa/paneth/SMx  
 # rhf/6-31g(d) iop(5/40=3000)

transition state, water, Gs(liq) -473.307482025

0 1

C					
C	1	1.346829			
N	2	1.351860	1	121.361649	
C	3	1.351859	2	120.586397	1
C	4	1.346830	3	121.361689	2
C	1	1.436466	2	120.725463	3
C	6	1.389753	1	122.348047	2
C	7	2.155022	6	99.295074	1
O	8	1.173803	7	104.345674	6
O	8	1.173803	7	104.346042	6
H	1	1.071791	2	119.502959	3
H	2	1.072944	1	122.539444	6
H	4	1.072944	3	116.098105	2
H	5	1.071791	4	119.502987	3
H	7	1.075820	6	118.355361	1
H	7	1.075819	6	118.355227	1
H	3	1.001845	2	119.704063	1

5\*\*\*\*\* ts-d \*\*\*\*\*

%SUBST I502 /home/paneth  
 %SUBST I701 /home/paneth  
 %SUBST I716 /home/paneth  
 # rhf/6-31g(d) iop(5/40=3000)

transition state, dioxan, Gs(liq) -473.299049460

0 1

C					
C	1	1.345606			
N	2	1.353708	1	121.325338	
C	3	1.353711	2	120.612846	1
C	4	1.345605	3	121.325323	2
C	1	1.436006	2	120.631887	3
C	6	1.392773	1	122.199687	2
C	7	2.031119	6	99.035979	1
O	8	1.179539	7	106.015760	6
O	8	1.179534	7	106.015251	6
H	1	1.071793	2	119.659198	3
H	2	1.072512	1	122.612370	6
H	4	1.072512	3	116.061936	2
H	5	1.071792	4	119.659349	3

H	7	1.075550	6	117.732445	1	-165.123286
H	7	1.075550	6	117.731776	1	-19.228387
H	3	0.998040	2	119.693487	1	-179.711269

6\*\*\*\*\* ts-g \*\*\*\*\*

#p rhf/6-31g(d)

transition state, gas phase: -473.2784659

0 1

C						
C	1	1.349576				
N	2	1.351928	1	121.000596		
C	3	1.351705	2	120.953509	1	0.881285
C	4	1.349432	3	120.983628	2	-0.876394
C	1	1.424224	2	120.290161	3	-0.443255
C	6	1.422438	1	121.589384	2	-173.333336
C	7	1.794258	6	99.840994	1	86.595683
O	8	1.199136	7	109.843913	6	89.243205
O	8	1.196893	7	109.515847	6	-89.347263
H	1	1.071497	2	119.936965	3	-178.435729
H	2	1.072056	1	122.900209	6	179.429409
H	4	1.072165	3	116.107581	2	179.007866
H	5	1.071382	4	119.923572	3	178.441955
H	7	1.076513	6	115.063117	1	-161.336453
H	7	1.077954	6	115.094203	1	-25.705094
H	3	0.995302	2	119.525692	1	179.543962

7\*\*\*\*\* z-aq \*\*\*\*\*

%SUBST 1502 /home/smpa/paneth/SMx  
 %SUBST 1701 /home/smpa/paneth/SMx  
 %SUBST 1716 /home/smpa/paneth/SMx  
 # rhf/6-31g(d) iop(5/40=3000)

zwitterion, water, Gs(liq): -473.354311523

0 1

C						
C	1	1.364629				
N	2	1.336487	1	119.967960		
C	3	1.331223	2	122.552569	1	-0.138155
C	4	1.370031	3	119.822106	2	-0.071599
C	5	1.393216	4	119.749745	3	0.205154
C	6	1.503838	5	120.548575	4	-178.351455
C	7	1.541566	6	115.269623	5	-106.391040
O	8	1.242648	7	114.674903	6	158.525697
O	8	1.238269	7	117.174034	6	-23.240284
H	1	1.069600	2	119.667592	3	-179.374533
H	2	1.072807	1	123.413621	6	-179.485533
H	4	1.073127	3	116.822634	2	-179.559316

H	5	1.071683	4	119.286244	3	-179.365752
H	7	1.081542	6	110.710698	5	16.994309
H	7	1.086918	6	109.169309	5	133.986587
H	3	1.008992	2	118.716892	1	-179.558872

8\*\*\*\*\* z-d \*\*\*\*\*

%SUBST 1502 /home/paneth  
 %SUBST 1701 /home/paneth  
 %SUBST 1716 /home/paneth  
 # rhf/6-31g(d) iop(5/40=3000)

zwitterion, dioxan, Gs(liq) -473.319634756

0 1

C						
C	1	1.360611				
N	2	1.341398	1	120.275252		
C	3	1.334176	2	122.189115	1	-0.003076
C	4	1.366252	3	119.988520	2	-0.197446
C	5	1.398599	4	119.981598	3	0.377541
C	6	1.492783	5	120.971991	4	178.884813
C	7	1.568401	6	112.507124	5	-109.765511
O	8	1.226777	7	114.417435	6	142.610739
O	8	1.233233	7	114.977126	6	-39.008864
H	1	1.068923	2	120.054716	3	-178.049226
H	2	1.071976	1	123.271536	6	179.780495
H	4	1.072227	3	116.720945	2	179.985706
H	5	1.072061	4	119.387121	3	179.950286
H	7	1.080261	6	111.115230	5	13.319709
H	7	1.086509	6	109.155134	5	132.488471
H	3	1.002851	2	118.864335	1	179.807996

9\*\*\*\*\* z-g \*\*\*\*\*

# rhf/6-31g(d)

zwitterion, gas phase: -473.2792583

0 1

C						
C	1	1.354583				
N	2	1.349587	1	120.687721		
C	3	1.341149	2	121.526341	1	0.433557
C	4	1.359806	3	120.398363	2	-0.537192
C	5	1.408493	4	120.241223	3	0.456123
C	6	1.464386	5	121.689199	4	175.455847
C	7	1.641142	6	108.206439	5	-105.788161
O	8	1.208736	7	112.977213	6	130.526056
O	8	1.222091	7	112.245371	6	-50.272883
H	1	1.069229	2	120.381317	3	-176.933326
H	2	1.071806	1	123.171404	6	179.115264

H	4	1.072110	3	116.431857	2	179.525924
H	5	1.072287	4	119.506475	3	179.425973
H	7	1.079140	6	112.410854	5	15.670249
H	7	1.083916	6	110.927213	5	139.852116
H	3	0.997047	2	119.178623	1	179.335518