Supporting Information for

Effect of Ammonium Salts on the Decarboxylation of Oxaloacetic Acid in Atmospheric Particles

Alexandra L. Klodt, Kimberly Zhang, Michael W. Olsen, Jorge L. Fernandez, Filipp Furche, and Sergey A. Nizkorodov

Department of Chemistry, University of California, Irvine, CA 92697, USA

Contents

Individual Experiment Data

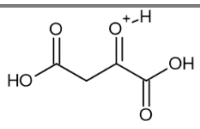
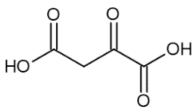
Table S1. Data from individual decarboxylation experiments: type of salt added to experimental solution, the concentration of salt added, measured solution pH, calculated rate constant from pseudo-first-order fit (as well as the fit's standard deviation), lifetime of OAA in this solution, and branching ratio to compare lifetime of OAA with respect to OH-oxidation and decarboxylation. The concentration of OAA was approximately 1 mM in all solutions. The branching ratio is calculated as $Q = \frac{\tau_d}{\tau_{OH}} = \frac{k_{OH}[OH]}{k_d}$, where t_d is the lifetime with respect to decarboxylation and k_{OH} is the rate constant for reaction with OH, so smaller (Q<1) values suggest decarboxylation is the faster process for those conditions. Branching ratios are calculated at pH 3.7 for all conditions except solutions containing ammonium bisulfate, which are calculated at pH 1.

Salt Added	Salt Concentration (M)	pH	Rate Constant ± 1 Standard Deviation (s^{-1})	Lifetime (h)	Branching Ratio (Q)
None	0		$(4.57 \pm 0.01) \times 10^{-5}$	6.1	6.53×10^{-3}
None	0	3.1	$(5.91 \pm 0.15) \times 10^{-5}$	4.7	5.05×10^{-3}
$(NH_4)_2SO_4$	0.10		$(8.75 \pm 0.03) \times 10^{-5}$	3.2	3.41×10^{-3}
$(NH_4)_2SO_4$	0.25	3.9	$(8.19 \pm 0.10) \times 10^{-5}$	3.4	3.65×10^{-3}
$(NH_4)_2SO_4$	0.50	3.9	$(1.24 \pm 0.02) \times 10^{-4}$	2.2	2.40×10^{-3}
$(NH_4)_2SO_4$	0.50		$(1.54 \pm 0.01) \times 10^{-4}$	1.8	1.94×10^{-3}
$(NH_4)_2SO_4$	0.75	3.5	$(1.45 \pm 0.02) \times 10^{-4}$	1.9	2.06×10^{-3}
$(NH_4)_2SO_4$	1.0	4.0	$(1.86 \pm 0.01) \times 10^{-4}$	1.5	1.60×10^{-3}
$(NH_4)_2SO_4$	1.0	4.0	$(1.89 \pm 0.02) \times 10^{-4}$	1.5	1.58×10^{-3}
$(NH_4)_2SO_4$	1.35	3.5	$(2.54 \pm 0.01) \times 10^{-4}$	1.1	1.17×10^{-3}
$(NH_4)_2SO_4$	1.48	3.7	$(2.52 \pm 0.02) \times 10^{-4}$	1.1	1.19×10^{-3}
$(NH_4)_2SO_4$	1.5	4.0	$(2.39 \pm 0.04) \times 10^{-4}$	1.2	1.25×10^{-3}
$(NH_4)_2SO_4$	1.85	3.8	$(2.53 \pm 0.02) \times 10^{-4}$	1.1	1.18×10^{-3}
$(NH_4)_2SO_4$	2.0	4.0	$(2.70 \pm 0.03) \times 10^{-4}$	1.0	1.10×10^{-3}
$(NH_4)_2SO_4$	2.25	3.9	$(2.63 \pm 0.02) \times 10^{-4}$	1.1	1.13×10^{-3}

$(NH_4)_2SO_4$	2.5	4.0	$(2.32 \pm 0.01) \times 10^{-4}$	1.2	1.29×10^{-3}
NH_4Cl	0.25	3.1	$(6.92 \pm 0.12) \times 10^{-5}$	4.0	4.31×10^{-3}
NH_4Cl	0.5	3.0	$(7.38 \pm 0.10) \times 10^{-5}$	3.8	4.04×10^{-3}
NH_4Cl	1.0	3.0	$(9.11 \pm 0.16) \times 10^{-5}$	3.1	3.28×10^{-3}
NH_4Cl	1.5	2.9	$(1.57 \pm 0.01) \times 10^{-4}$	1.8	1.90×10^{-3}
NH_4Cl	2.0	2.9	$(1.97 \pm 0.09) \times 10^{-4}$	1.4	1.51×10^{-3}
NH_4Cl	2.5	2.7	$(2.35 \pm 0.01) \times 10^{-4}$	1.2	1.27×10^{-3}
NH_4HSO_4	0.5	1.3	$(8.05 \pm 0.12) \times 10^{-6}$	35.5	4.23×10^{-2}
NH_4HSO_4	0.8	1.0	$(6.15 \pm 0.10) \times 10^{-6}$	45.2	5.54×10^{-2}
NH_4HSO_4	1.5	0.4	$(4.49 \pm 0.03) \times 10^{-6}$	62.0	7.60×10^{-2}
NH_4HSO_4	2.0	0.2	$(2.37 \pm 0.04) \times 10^{-6}$	117	1.44×10^{-1}
H_2SO_4	0	1.0	$(4.36 \pm 0.04) \times 10^{-6}$	63.7	7.82×10^{-2}
Na_2SO_4	0.25	3.5	$(5.83 \pm 0.05) \times 10^{-5}$	4.8	5.11×10^{-3}
Na_2SO_4	0.75	3.4	$(3.55 \pm 0.10) \times 10^{-5}$	7.8	8.39×10^{-3}
Na_2SO_4	1.0	3.4	$(5.44 \pm 0.04) \times 10^{-5}$	5.1	5.48×10^{-3}
Na_2SO_4	1.34	3.6	$(4.94 \pm 0.03) \times 10^{-5}$	5.6	6.03×10^{-3}

Equilibrium Ratios of OAA's Forms in Solution

Table S2. The possible forms OAA takes in solution and the abundances as determined by Kozlowski et al.[1]

Structure	pH 3.7 (%)	pH 1 (%)
 Protonated keto form	0	3.4
 H_2A keto form	0.2	10.6

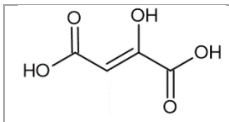
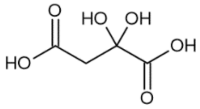
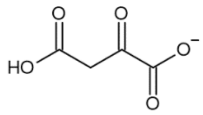
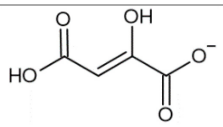
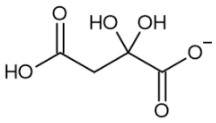
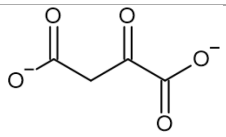
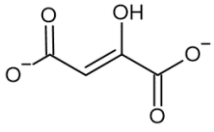
 H_2A enol form	0.4	3.4
 H_2A gem-diol form	1.3	75.5
 HA^- keto form	45.5	4.6
 HA^- enol form	5.9	0.6
 HA^- gem-diol form	19	1.9
 A^{2-} keto form	24	0
 A^{2-} enol form	3.2	0

Table S3. Values used to calculate OH rate constants. The protonated keto form could not be included in the calculation of the OH-oxidation rate constants, so values from Table S2 were renormalized to exclude it from the calculation. We do not expect this to have a significant effect on the calculated OH-oxidation rate as the keto forms generally react an order of magnitude more slowly than the gem-diol forms,[2] and the protonated keto form only accounts for 3.4% of the abundance at pH 1 and is not present at pH 3.7.[1] OH-oxidation rate constants for the enol forms of OAA were also not calculable using the SAR.[3,4] However, but-2-enedioic acid, which

has the same structure as enol OAA with the exception of enol OAA's vinylic alcohol group, reacts quickly with the OH radical (6×10^9 M^{-1} s^{-1}; see fumaric acid and maleic acid in Buxton et al.[5]). Additionally, but-2-enedioic acid only has two equivalent hydrogens which may be abstracted by OH, so the reactivity of each hydrogen should be half of but-2-enedioic acid's total OH reactivity, or 3×10^9 M^{-1} s^{-1}. We therefore assumed the OH reactivity of enol OAA's vinylic hydrogen to be equivalent to the reactivity of one of but-2-enedioic acid's vinylic hydrogens and the OH reactivity of enol OAA's vinylic alcohol group to be 6.9×10^7 M^{-1} s^{-1}, which is the base value for alcohol groups in the SAR.[3]

Form	OH-oxidation rate constant ($M^{-1}s^{-1}$)	Ratio used for pH 3.7 (%)	Ratio used for pH 1 (%)
H_2A keto form	7.01×10^6	0.2	11.0
H_2A enol form	3.07×10^9	0.4	3.5
H_2A gem-diol form	2.61×10^8	1.3	78.2
HA^- keto form	1.23×10^7	45.5	4.8
HA^- enol form	3.07×10^9	5.9	0.6
HA^- gem-diol form	4.51×10^8	19.0	2.0
A^{2-} keto form	4.22×10^7	24	0
A^{2-} enol form	3.07×10^9	3.2	0
Final rate constant for OH oxidation		**2.98×10^8 $M^{-1}s^{-1}$**	**3.41×10^8 $M^{-1}s^{-1}$**

Sample Kinetics Fits for Decarboxylation Reaction

When monitoring the decarboxylation of OAA by UV-Vis, it can be seen (Figures S1-S3) that the decrease at 260 nm is not strictly a first-order decay until after some time has passed, corresponding to the keto/enol and keto/gem-diol conversions both reaching equilibrium. Since the conversion between OAA's keto and gem-diol forms is faster in water than between the keto and enol forms,[6] it is likely the keto/enol interconversion that controls the change in the pre-equilibrium absorbance. However, to the best of our knowledge, the rate of keto/enol interconversion has not been determined at pH values smaller than 5 (although the keto/enol

equilibrium ratios are available[1]). At pH values above 5, the rate has been shown to be highly pH dependent,[6] so it would not be reasonable to apply rate constants obtained at higher pH values to our data. In any case, the expected first-order kinetics are observed after the solution has had time to reach keto/enol equilibrium. To avoid interference from the solution equilibration, we began fitting once the data had adopted a first-order decay pattern. The first point for the fit was chosen by performing sample fits beginning at each data point, then using the one with the earliest starting point with which the later fits agree within the standard deviation of the chosen fit. This difference is small under conditions of high ammonium concentration (0 to 5 percent), but much larger with low ammonium concentrations (5 to 10 percent) and/or high acidity (10 to 25 percent).

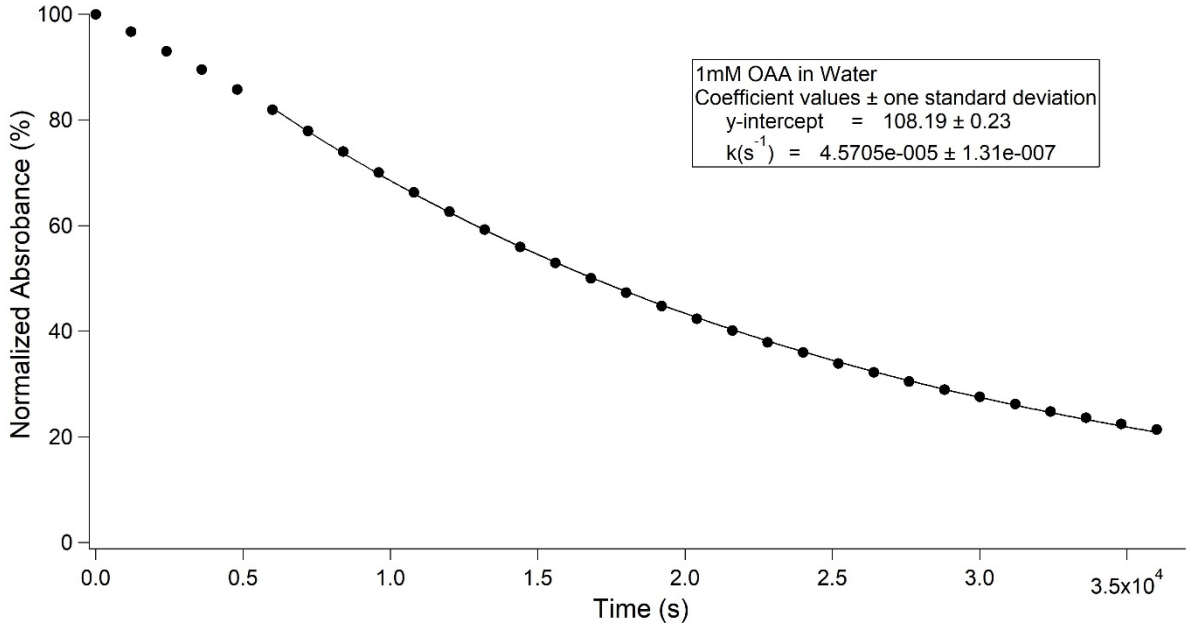


Figure S1. Absorbance at 260 nm, normalized to time 0, for 1 mM OAA in pure water. The data is shown with individual dots and the fit with a solid line.

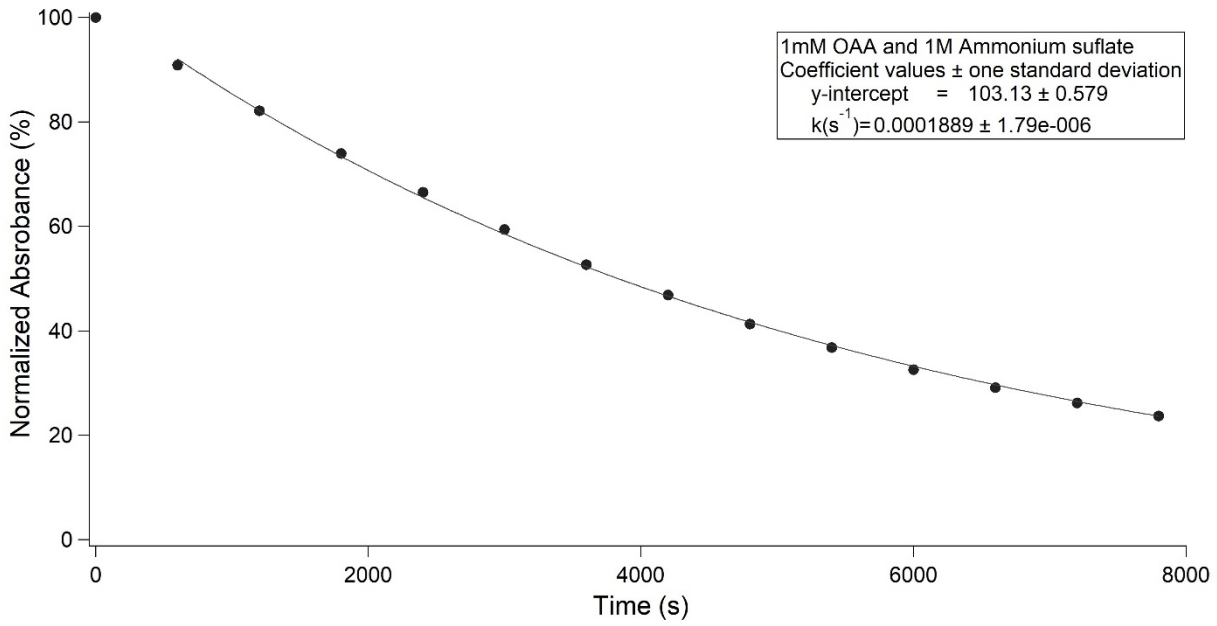


Figure S2. Absorbance at 260 nm, normalized to time 0, for 1 mM OAA in 1 M ammonium sulfate solution. The data is shown with individual dots and the fit with a solid line.

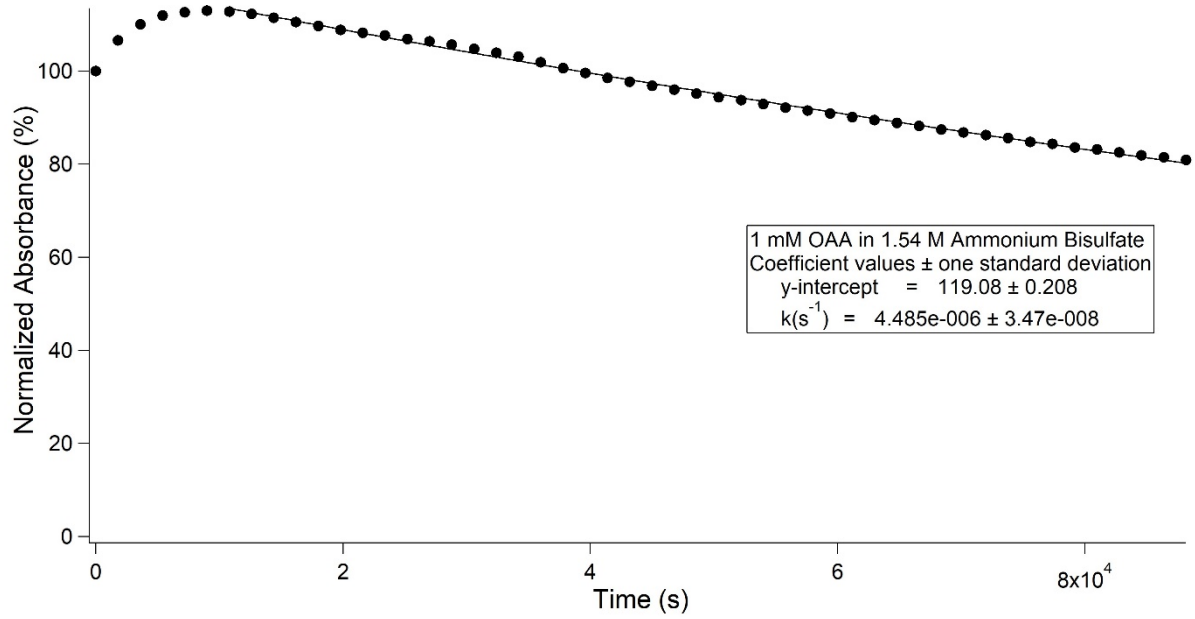


Figure S3. Absorbance at 260 nm, normalized to time 0, for 1 mM OAA in 1.54 M ammonium bisulfate solution. The data is shown with individual dots and the fit with a solid line.

Initial Absorbance Spectra for Each Salt System

Although all solutions were prepared at close to 1 mM concentrations of OAA as possible, the actual concentration of each solution was used to scale each spectrum by 1mM/(exact concentration) to make the peak heights more directly comparable in Figures below.

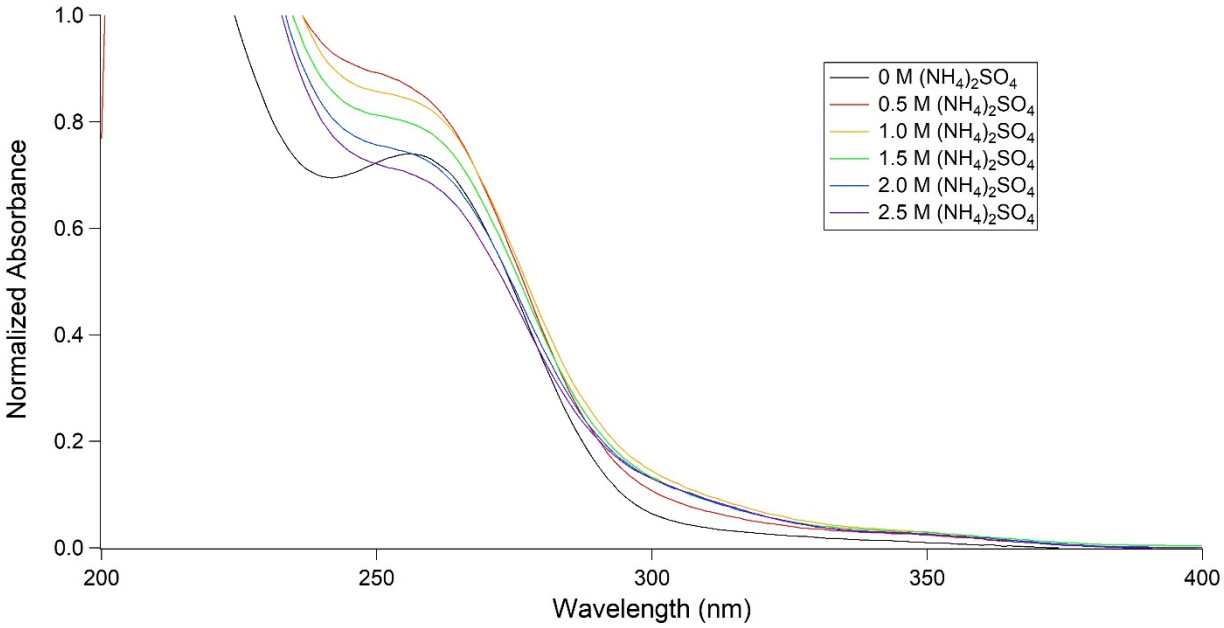


Figure S4. Initial absorbance spectra for solutions containing ammonium sulfate.

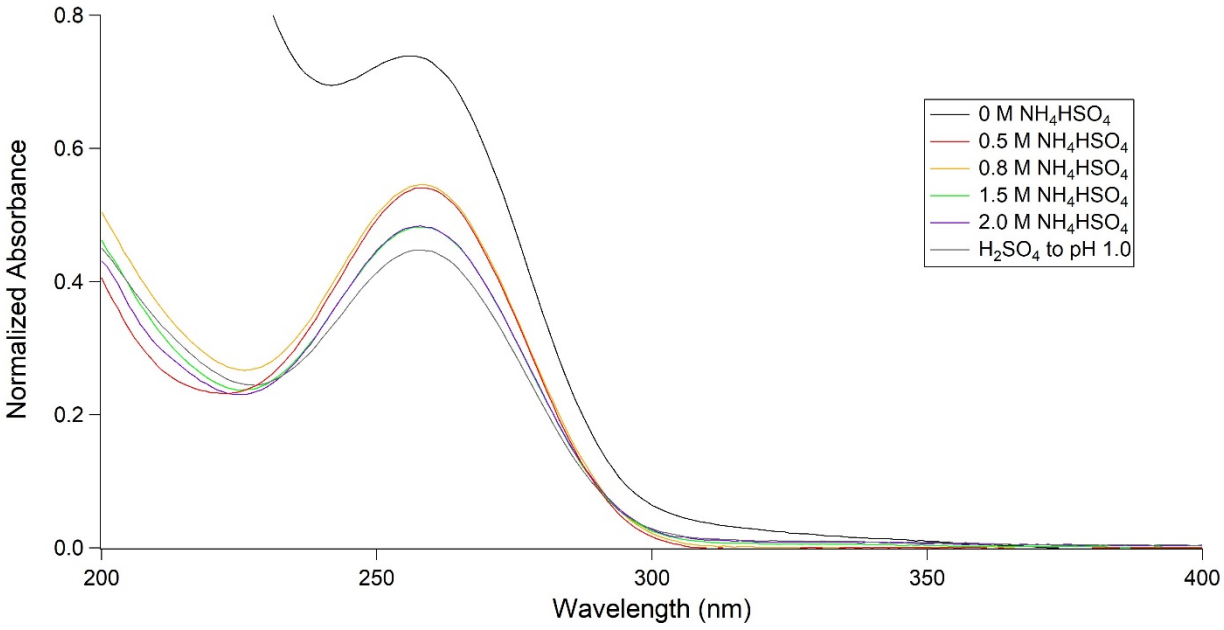


Figure S5. Absorbance spectra for OAA in ammonium bisulfate at their maximum value.

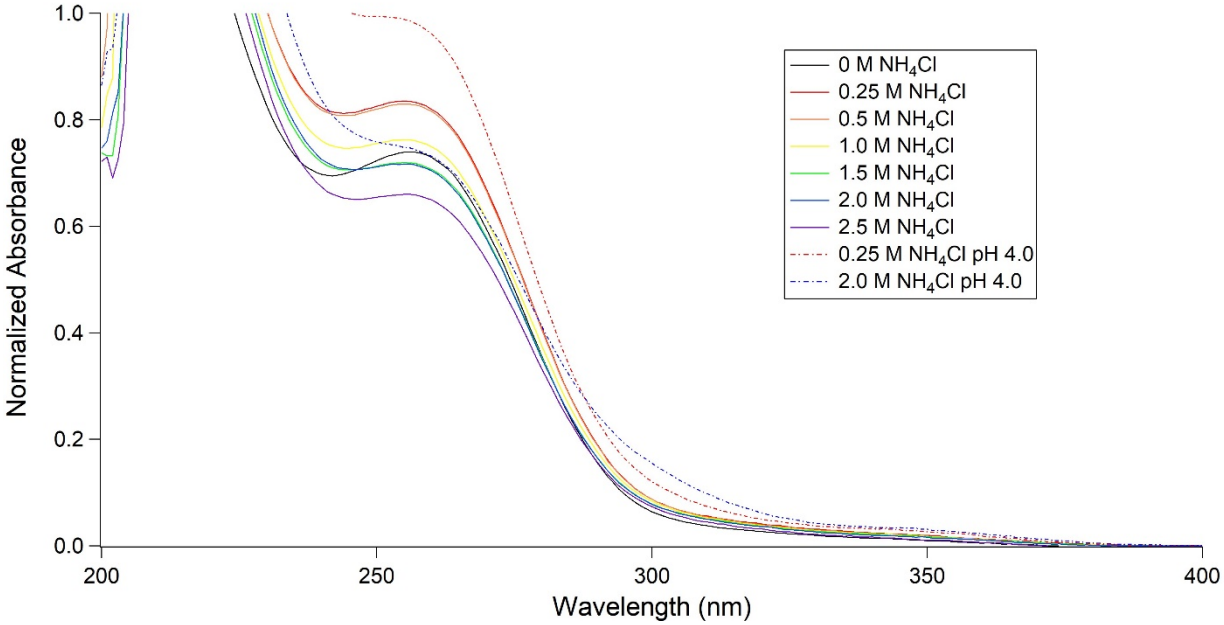


Figure S6. Initial absorbance spectra for solutions containing ammonium chloride. The traces in dashed lines have the pH adjusted to 4.0 so that the enol band is present as in the ammonium sulfate conditions.

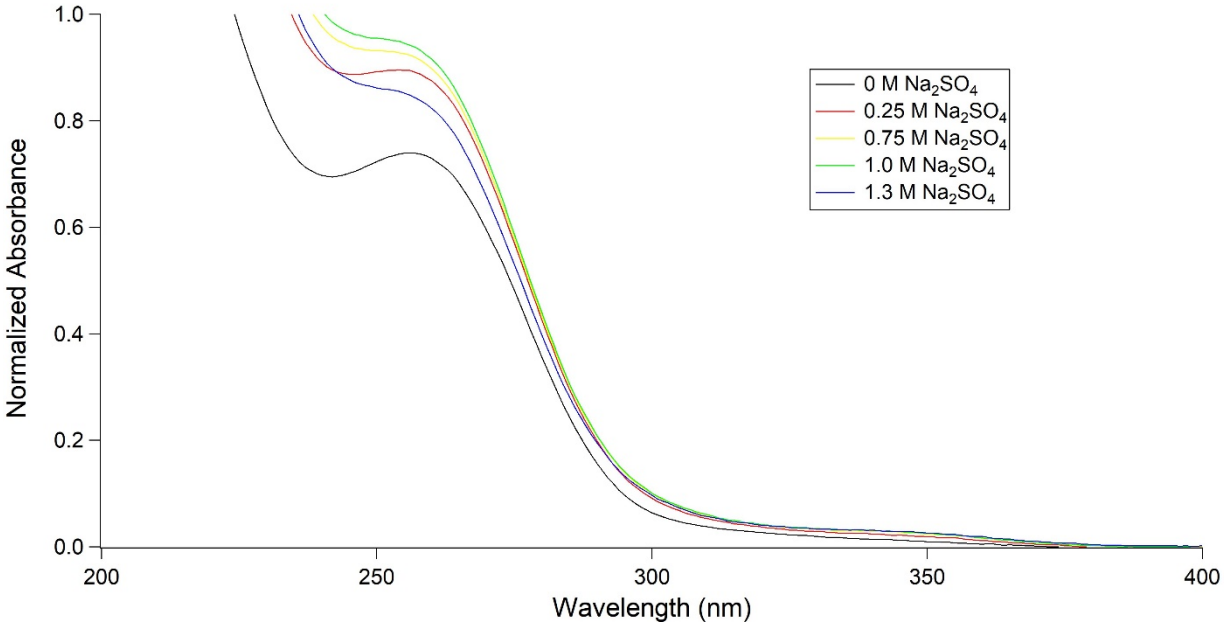
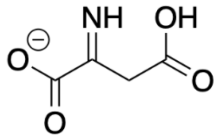


Figure S7. Initial absorbance spectra for solutions containing sodium sulfate.

Coordinate Files for Optimized Geometries of Deprotonated Imine



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With COSMO

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2.59261394688963 0.83141153945583 -0.02457943271809 c
0.18028088307231 -1.91646002091955 -1.66689517115228 h
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-2.31527212246562 3.16291382864154 0.01427597658222 n
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4.61721802993885 -0.24397932950426 -0.04652385769604 o
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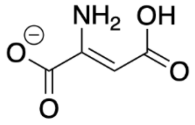
Coordinate Files for Optimized Geometries of Deprotonated Enamine



Without COSMO

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   -3.38839674867898     2.79773078243661    -0.85999660847036  n
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    1.65784382168735     1.72361874683273    -1.00258072947519  o
    2.90210971080549    -2.16350683783555     0.03481418541245  o
   -6.54773202742642    -2.68735921569896     1.05742131104828  o
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With COSMO

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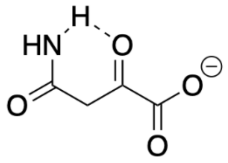
Coordinate Files for Optimized Geometries of Catalyzed Decarboxylation Transition State



Without COSMO

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    0.42927336507091    -3.54738202817216     0.37373441114186  h
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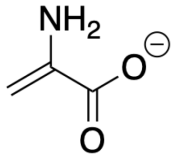
    4.22997368187346     1.70893459802325    -0.43302726063385  o
   -2.20790418838354     3.58043259047400     0.40299705012911  h
    0.87811125030310     3.23366982387751     1.67914173737672  h
$end
```

With COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -510.3142144989     508.2321731367    -1018.546387636
    21 -510.3142599535     508.2602631873    -1018.574523141
$end
$coord
   -3.03427366688651    -0.76643828474428     0.20788879181380  c
   -1.03939457357870     0.96726068396646    -1.02283606918911  c
    0.90546224932917    -0.00356986021305    -2.44755634719791  c
    3.69285828077633    -0.29432570295772     0.44164344456781  c
    2.05094187905678     1.24819226439226    -3.59722429715666  h
    0.75141914790139    -1.95516626173509    -3.01437081803248  h
   -2.94656744421013    -3.04610726525747    -0.34459969292991  o
   -4.55407910764890     0.32498933115536     1.65002471961029  o
   -1.32282475657175     3.39310480756612    -0.47023784699543  n
    4.21299871542780    -2.47655302982087     0.51127127093896  o
    4.05129747804315     1.80501292306534     1.14742841362094  o
   -2.68511386709092     3.84081888423959     0.78401570305802  h
   -0.10928302499998     4.72270745696458    -1.07478144796341  h
$end
```

Coordinate Files for Optimized Geometries of Catalyzed Decarboxylation Intermediate



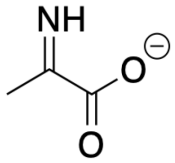
Without COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -321.7189111597     320.1485782980    -641.8674894577
    11 -321.7450882603     320.4612986593    -642.2063869196
$end
$coord
   -6.06464364938709    -0.53468554493112    -0.00000137843277  c
   -3.58173048211600     1.04273027045942    -0.00001435628898  c
   -1.28068079363292    -0.02709941714606    -0.00000511147927  c
   -4.08127242637692     3.56902225525004     0.00000088154673  n
   -1.16612945774178    -2.06467531254580    -0.00000049324144  h
    0.44844731675615     1.08225101863541     0.00000140187489  h
   -8.03301058742519     0.78824415348753    -0.00002060588175  o
   -5.84620862958625    -2.86397015643672     0.00001959120385  o
   -5.94876491229124     3.95981433765945     0.00001868495789  h
   -2.73233026199513     4.89200851355313     0.00000138574086  h
$end
```

With COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -321.8354956969     320.1674231425    -642.0029188393
    10 -321.8542154782     320.4877674691    -642.3419829473
$end
$coord
   -6.03352619679689    -0.54877804561190    -0.00011583452509  c
   -3.61763952141288     1.05513214557129    -0.00012676644241  c
   -1.31973373927497    -0.03059710566772    -0.00083078884260  c
   -4.07912302038535     3.58326764985491    -0.00049993534892  n
   -1.18754250542507    -2.06619153944276    -0.00083922929542  h
    0.40281560517282     1.07998139006151    -0.00150354918450  h
   -8.06904817776008     0.66489761895855    -0.00557547909084  o
   -5.79979154864590    -2.89435691121703     0.00507340129222  o
   -5.89504799800915     4.13173031543696     0.00265361475757  h
   -2.68768678125887     4.86855460004147     0.00176456667994  h
$end
```

Coordinate Files for Optimized Geometries of Catalyzed Decarboxylation Product



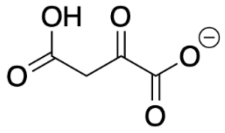
Without COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -321.7292603270     320.1981841977    -641.9274445247
    10 -321.7565695832     320.4775535500    -642.2341231333
$end
$coord
   -6.00785085947250     3.64406453019673    -0.00675559406776  c
   -3.42463877408778     5.05303154702654     0.00247983061051  c
   -1.07373895057244     3.48265518546369     0.00131340310631  c
   -1.06591126462617     2.22805868149981     1.64048218867222  h
    0.60080248156940     4.68669057906609     0.00828731966653  h
   -1.06015776043284     2.23909213891064    -1.64620509277910  h
   -3.30669309226137     7.44853401048599     0.01072556759664  n
   -7.89328205744320     5.05422813022262    -0.00520140432359  o
   -5.87001883863567     1.29477027007249    -0.01451980541862  o
   -5.16757936550019     8.01030208872290     0.00939358693682  h
$end
```

With COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -321.8384766030     320.2166066723    -642.0550832753
    10 -321.8590884559     320.5026825511    -642.3617710070
$end
$coord
   -5.98775408372597     3.65165076818780    -0.00675710392156  c
   -3.41666725484977     5.03828773035572     0.00303611847124  c
   -1.07314833002027     3.47722689252460     0.00050021480328  c
   -1.04371506076006     2.23198546863177     1.64618979363850  h
    0.59893167380359     4.67815341723597     0.00774979970246  h
   -1.03877028587727     2.24526282945070    -1.65512392902036  h
   -3.32817925613785     7.43523359196750     0.01283028185782  n
   -7.90360708971065     5.03250614407513    -0.01297882273285  o
   -5.91301237190218     1.29647980684953    -0.00732731654224  o
   -5.16314642228234     8.05464051238878     0.01188096374375  h
$end
```

Coordinate Files for Optimized Geometries of Deprotonated Oxaloacetic Acid



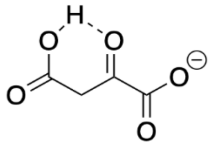
Without COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -530.0297541909     527.5074196714    -1057.537173862
    45 -530.1045271545     528.1354360043    -1058.239963159
$end
$coord
   -4.27925690580448    -1.02487277213909    -0.08767686213387  c
   -1.88586851542744     0.57356900623240    -0.19961144721638  c
    0.54112934754141    -0.86131389741863     0.29506639304730  c
    3.03143546275298     0.56348177854812     0.25162433320910  c
    0.64219882163677    -2.39692301252422    -1.08380750120346  h
    0.35806367912104    -1.80367600875511     2.12434816962884  h
    2.88471078525673     3.00082024754497    -0.28399988828257  o
    5.01496239167232    -0.47348395429110     0.67680522323942  o
   -5.28512325440048    -1.09915124764101     2.02517991359323  o
   -4.77608978125121    -2.07812850328982    -2.12242826389612  o
    1.03848287495585     3.39329392224995    -0.53711887901570  h
   -1.85931282580445     2.84592445663602    -0.67051490219500  o
$end
```

With COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -530.1352455991     527.4840650194    -1057.619310619
    57 -530.1996174736     528.1444484406    -1058.344065914
$end
$coord
   -4.27443766867239    -1.04827968043390    -0.04382395900774  c
   -1.86036730225126     0.51656354760708    -0.18587252536262  c
    0.57080471005614    -0.87438186599697     0.28318267894909  c
    3.01853656461352     0.60075196668801     0.23194757575507  c
    0.71089435627155    -2.39728272402729    -1.10979159226384  h
    0.43341228838345    -1.83826872198742     2.10692225302715  h
    2.87248201961391     3.03013128990328    -0.31203874319458  o
    5.02380920804457    -0.40095516005268     0.66382913794745  o
   -5.34305692195763    -1.04857475669105     2.04658569080676  o
   -4.85517731753431    -2.13640280748665    -2.04290047320715  o
    1.05833608328486     3.46053184246479    -0.57608083365605  h
   -1.92990393960336     2.77570708516518    -0.67409292101872  o
$end
```

Coordinate Files for Optimized Geometries of Uncatalyzed Decarboxylation Transition State



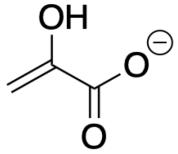
Without COSMO

```
$energy      SCF             SCFKIN          SCFPOT
    1 -530.0450625309     527.6086371147    -1057.653699646
   62 -530.0577409784     527.8465879239    -1057.904328902
$end
$coord
  -3.93293222139808    -0.24748122384297     0.26635480020379  c
  -1.17794198229385     0.37338054852618    -0.30649059240391  c
   0.66260061953111    -1.74802808036896    -0.23749116320631  c
   4.13071418158366    -0.40817810761207     0.44164999945593  c
   0.90412811389642    -2.57679119162057    -2.10771128125337  h
   0.24852548554602    -3.17993111991076     1.17039498026022  h
   4.14073406888186     1.99967370097528     0.02976876698887  o
   5.81534935617802    -1.75704847607465     1.05837969141626  o
  -4.27948191074677    -0.43484181708550     2.58184425723923  o
  -5.33917938186392    -0.53088503873973    -1.57594733922257  o
   2.28466207268850     2.48846812265245    -0.42198200554477  h
  -0.43887207395532     2.54319398357216    -0.77155615885072  o
$end
```

With COSMO

```
$energy      SCF             SCFKIN          SCFPOT
    1 -530.1425614117     527.8549779781    -1057.997539390
   71 -530.1425628306     527.8701542930    -1058.012717124
$end
$coord
  -3.69319402159054    -0.49356695131291     0.22796841918397  c
  -1.14917559810936     0.64593410566187    -0.48524387114702  c
   0.63111270631076    -0.84471748303088    -1.96918412737252  c
   4.02004571247071    -0.40493483932685    -0.04632768061470  c
   1.22620796954637     0.08733292058833    -3.70286330890529  h
   0.25446925162370    -2.84647147802345    -2.16717250772574  h
   4.00983237192440     1.79769599772889     0.96505873183049  o
   5.58590972270708    -1.99830634353051    -0.09783389516654  o
  -3.56072929488055    -2.12704951111625     1.91597758563893  o
  -5.56511204229214     0.31490504927729    -0.93518324931087  o
   2.25573611804102     2.58206283089047     0.66702682731240  h
  -0.56578476596594     2.78677978450797     0.27280225915857  o
$end
```

Coordinate Files for Optimized Geometries of Uncatalyzed Decarboxylation Intermediate



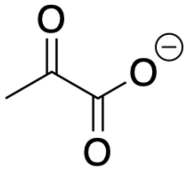
Without COSMO

$energy SCF SCFKIN SCFPOT
1 -341.5897095674 340.1266176292 -681.7163271966
13 -341.6240598518 340.3133673526 -681.9374272044
$end
$coord
-4.34884724771373 -2.93625653164959 -0.09263753776147 c
-2.17655424229989 -0.99470702779651 -0.01294304629221 c
0.27819033969752 -1.56307245545124 -0.11661582949476 c
0.80325716358594 -3.52989426317681 -0.26802055388390 h
1.72551975603691 -0.11489614708325 -0.05300309406167 h
-3.10564633222349 1.36069280992683 0.17631988305860 o
-6.46876298147314 -1.83655953471010 0.03713572612857 o
-3.86490686562413 -5.20765706157978 -0.26233394300986 o
-4.94535571423761 0.90916596910460 0.19168432501952 h
$end

With COSMO

$energy SCF SCFKIN SCFPOT
1 -341.6995770143 340.1513421545 -681.8509191688
12 -341.7224569113 340.3450131645 -682.0674700759
$end
$coord
-4.33396839036417 -2.94614610061270 -0.09372351904245 c
-2.19970449276889 -1.01199087886447 -0.01326569820195 c
0.24970175578718 -1.58008271179576 -0.11716532613140 c
0.80154499876326 -3.53897431091672 -0.26881906131436 h
1.69467954267732 -0.13170104435523 -0.05341666008015 h
-3.08362559475712 1.37380452081466 0.17682317629093 o
-6.49284019444859 -1.94832424612322 0.02955902675874 o
-3.82036239466945 -5.22804408823156 -0.26461675127167 o
-4.91853135447119 1.09827461766917 0.20421074269512 h
$end

Coordinate Files for Optimized Geometries of Uncatalyzed Decarboxylation Product



Without COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -341.5972811121     340.1835117557    -681.7807928678
    33 -341.6241347550     340.3385371933    -681.9626719483
$end
$coord
   -1.17942299968227    -2.13770291470677    -1.10008444703973  c
    0.41869123709948    -0.02057213746003     0.06415927392776  c
    2.64377775773625    -0.94660175430437     1.61118158206846  c
    1.94572628345406    -2.15686884973015     3.13160035698809  h
    3.70454255275967     0.64350455438844     2.38507067138711  h
    3.85709977469878    -2.10831693326866     0.41054705113886  h
    0.00824014793949     2.22494725108042    -0.18382106605208  o
   -2.92263258854826    -2.90576231061702     0.27631690711444  o
   -0.44156805257392    -2.85359414255369    -3.21379674352865  o
$end
```

With COSMO

```
$energy      SCF             SCFKIN          SCFPOT
     1 -341.5972811121     340.1835117557    -681.7807928678
    44 -341.7301637246     340.3674969094    -682.0976606340
$end
$coord
   -1.17555280574825    -2.12675765235991    -1.09794462436673  c
    0.46280567812465    -0.07080563201803     0.09229395531265  c
    2.66986952283871    -0.93777337528771     1.63078704829743  c
    2.00071694240394    -2.14626428070203     3.16654272758189  h
    3.71083617846387     0.66584383744154     2.39248862592769  h
    3.90993600803669    -2.09768917448241     0.45462761575647  h
   -0.03916616044384     2.15300330901328    -0.22253309506811  o
   -2.98169756910907    -2.87518721942293     0.21571435827872  o
   -0.52329368168344    -2.82533704935367    -3.25080302571575  o
$end
```

Coordinate Files for Optimized Geometries of Carbon Dioxide

Without COSMO

```
$energy      SCF            SCFKIN          SCFPOT
     1 -188.4770559969     187.6153602092    -376.0924162061
    11 -188.4792997339     187.8206011469    -376.2999008808
$end
$coord
  -0.79870713486122     3.48581060521619     0.78908068363827  c
   1.05929405167456     4.62384666540040     1.17867975137030  o
  -2.65670296143107     2.34776589490544     0.39948059429985  o
$end
```

With COSMO

```
$energy      SCF            SCFKIN          SCFPOT
     1 -188.4770559969     187.6153602092    -376.0924162061
    16 -188.4821808758     187.8116710016    -376.2938518774
$end
$coord
  -0.79870493454483     3.48580765735266     0.78908037269294  c
   1.05834231137275     4.62326586578329     1.17848056956138  o
  -2.65575342144612     2.34834964238811     0.39968008705457  o
$end
```

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(2) Merz, J. H.; Waters, W. A. Some Oxidations Involving the Free Hydroxyl Radical. *J. Chem. Soc.* **1949**, S15–S25.

(3) Monod, A.; Doussin, J. F. Structure-Activity Relationship for the Estimation of OH-Oxidation Rate Constants of Aliphatic Organic Compounds in the Aqueous Phase: Alkanes, Alcohols, Organic Acids and Bases. *Atmos. Environ.* **2008**, *42* (33), 7611–7622. https://doi.org/10.1016/j.atmosenv.2008.06.005.

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