SUPPORTING INFORMATION

Concert along the Edge: Dynamics and the Nature of the Border between General and Specific Acid–Base Catalysis

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Experimental Procedures

Natural Abundance Isotope Effects

Synthesis of Benzoylacetic Acid (**1**). Example Procedure: A mixture of 13.5 mL (15 g, 78 mmol) of ethyl benzoylacetate and 150 mL (133 mmol) of 0.89 N aqueous KOH was stirred at ambient temperature for 24.5 h. The aqueous layer was then washed with four 50-mL portions of ether (to remove unreacted ethyl benzoylacetate), then cooled to 0 °C and acidified by the dropwise addition of 20% sulfuric acid until acidic by litmus paper. A white precipitate formed and was collected by vacuum filtration, then the solid was allowed to dry overnight at 25 °C to afford 9.39 g of solid. The solid was redissolved in a minimum amount of ether, ~500 mL, at room temperature, then 250 mL of toluene was added. The resulting mixture was cooled in an ice-water bath, then slowly concentrated on a rotary evaporator until the volume was reduced by about two-thirds and a solid started to form. The resulting mixture was cooled to 0 °C overnight, vacuum filtered, and air-dried overnight to afford 5.85 g (46%) of benzoylacetic acid.

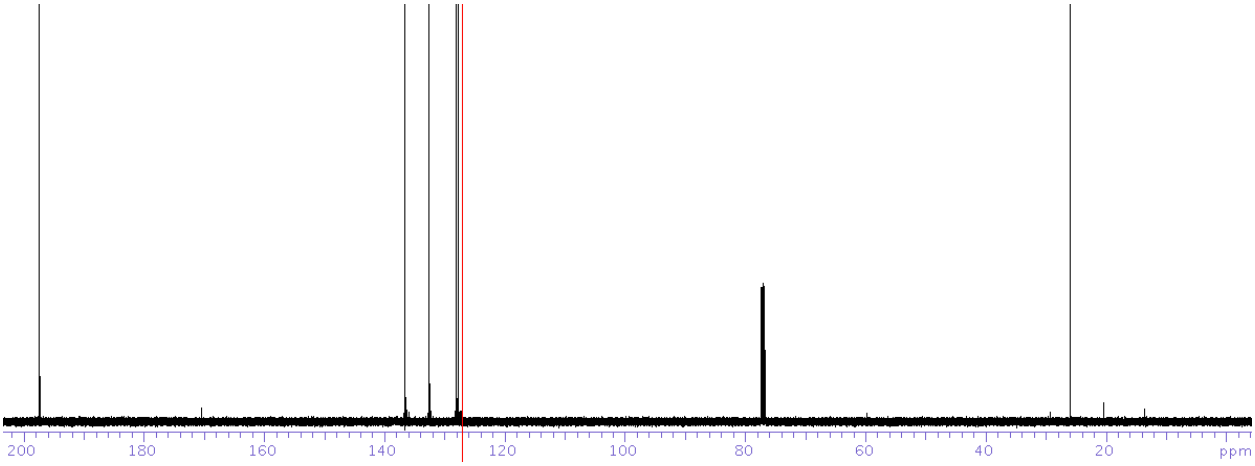
Low-conversion Decarboxylation of Benzoylacetic Acid (**1**). Example Procedure: A mixture of 4.85 g (26.3 mmol) of **1**, 600 mL of dichloromethane, and 0.843 g of benzyl ether (internal standard) was stirred for 9 h at 25 °C, and the conversion was judged to be 15.6% by NMR analysis of an aliquot. The reaction mixture was diluted with 1200 mL of ethyl and rinsed successively with two 850-mL portions of saturated aqueous $NaHCO_3$. The organic layer was concentrated on a rotary evaporator, and the residue was chromatographed on a 1 inch X 8 inch silica gel column using 10% ethyl acetate in hexanes as eluent to afford 300 mg of acetophenone for analysis.

100%-Conversion Decarboxylation of Benzoylacetic Acid (**1**). Example Procedure: A sample of 1.00 g of **1** was warmed gently until it liquefied and all apparent evolution of CO_2 stopped.

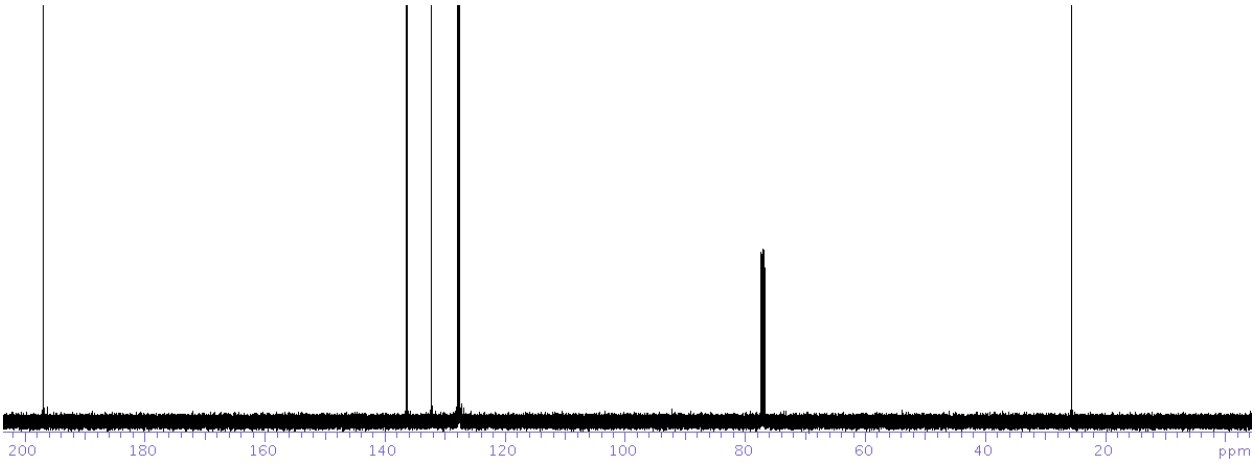
NMR Measurements

^{13}C NMR Spectrum of Sample (15.6% conversion), Experiment 1.

A note on spectra: we certify that all spectra presented are unaltered screen dumps or pdf printouts of the original spectra. Please note that scales are typically increased by a factor of 5 from normal to show impurities clearly. The raw electronic files are saved and always available on request.



^{13}C NMR Spectrum of Standard (100% conversion) for Experiment 1



All NMR samples consisted of approximately 400 mg of acetophenone in a 5 mm NMR tubes filled to a constant height of 5 cm with $CDCl_3$. The ^{13}C spectra were recorded at 125.7 MHz using inverse gated decoupling, 100 s delays between calibrated 46° pulses, and a 7 s acquisition time to collect 448718 points. The integrations were obtained numerically by a procedure given in a macro provided in a later section. A zero-order baseline correction was generally applied, but to avoid any qualitative manipulation no first-order or higher-order baseline correction was ever applied. Six spectra were recorded for each sample and standard.

NMR Results and Calculation of KIEs

The raw integrations are shown in Table S1, along with average values and standard deviations. The integration of peak 4, the meta ring carbon, was in each case set to 2000. The numbers are in order from left to right in the spectrum of acetophenone, corresponding to the carbonyl, ipso, para, meta, ortho, and methyl carbons, respectively.

Table S1.

	macro used: hstd1						
Standard1	File: standard_100_percent_conversion_spectra.fid					average	stdev
1001.2	1003.0	1000.9	1001.9	1007.2	999.2	1002.2	2.8
996.7	996.9	993.3	995.7	991.7	996.2	995.1	2.1
996.0	995.1	993.4	992.7	991.3	992.1	993.4	1.8

2000.0	2000.0	2000.0	2000.0	2000.0	2000.0	2000.0	0.0
2032.1	2028.7	2023.2	2026.2	2029.1	2025.1	2027.4	3.2
969.1	970.5	968.9	972.4	974.2	968.6	970.6	2.2

macro used: hsam1

Sample1	File: 20_percent_conversion_spectra.fid					average	stdev
995.3	996.5	999.0	995.0	999.0	1000.5	997.6	2.3
990.8	995.2	993.2	991.2	993.1	987.6	991.9	2.6
997.5	993.9	989.9	992.7	993.4	996.0	993.9	2.6
2000.0	2000.0	2000.0	2000.0	2000.0	2000.0	2000.0	0.0
2030.2	2024.6	2027.8	2024.3	2026.7	2028.5	2027.0	2.3
937.3	933.4	933.7	934.7	937.3	937.1	935.6	1.9

macro used: hstd3

Standard2	File: KIE3-100percentconversionspectra-08292013-HRA.fid					average	stdev
1004.0	1002.7	1006.7	1004.8	1008.9	1005.7	1005.4	2.2
987.1	991.0	988.6	987.2	988.0	991.2	988.9	1.8
996.5	996.2	995.0	997.8	998.6	996.8	996.8	1.3
2000.0	2000.0	2000.0	2000.0	2000.0	2000.0	2000.0	0.0
2015.6	2016.5	2021.4	2015.8	2023.3	2020.7	2018.9	3.3
966.0	965.0	963.7	962.6	965.8	967.7	965.1	1.8

macro used: hsam3

Sample2	File: KIE3-20percentconversionspectra-08312013-HRA.fid					average	stdev
1001.3	999.5	1000.5	1005.6	996.1	1002.1	1000.8	3.1
989.0	987.2	987.5	991.7	990.6	989.0	989.2	1.8
993.5	996.1	997.7	998.5	993.5	996.4	995.9	2.1
2000.0	2000.0	2000.0	2000.0	2000.0	2000.0	2000.0	0.0
2026.7	2024.1	2026.4	2023.8	2025.9	2024.4	2025.2	1.3
933.8	934.4	931.7	929.3	934.3	925.7	931.5	3.5

The isotope effects in the main text were then calculated as:

KIE = ln(1-F)/ln(1-(F*IntSample/IntStandard))

where F is the fractional conversion (0.156 for reaction 1, 0.184 for reaction 2), IntSample is the average integration for the sample for the carbon peak of interest in the table above, and IntStandard is the average integration for standard for the carbon peak of interest in the table above. For example, the KIE for carbon 1 of sample 2 /standard 2 was calculated as ln(1-0.184)/ln(1-0.184*1000.8.0/1005.4).

The uncertainties arising from uncertainties in F were negligible, and the major source of uncertainty is random variation in the integrations due to noise. For six measurements, the 95% confidence ranges in the average raw integrations are approximately the standard deviations shown in the table above, and the 95% confidence ranges for the KIEs were approximated as the square-root of the sum of the squares of the fraction uncertainties in the integrations.

H/D Isotope Effect by Absolute Kinetics

Deuterated Aqueous Phosphoric Acid. To 2.83 g (20 mmol) of P_2O_5 at 0 °C under N_2 was added slowly 3 mL (3 g, 150 mmol) of 99.9% D_2O. The resulting mixture was stirred for 1 h then diluted to 10.0 mL using additional D_2O.

Deuterated Benzoylacetic Acid (**1**-d_3). To a mixture of 0.5 g (3 mmol) of **1** in 5 mL of D_2O was added 0.159 g (1.5 mmol) of Na_2CO_3, and the mixture was stirred for 10 min. The mixture was then reacidified using 0.75 mL (3 mmol) of the deuterated aqueous phosphoric acid solution generated above. The solid precipitate was then collected by filtration under N_2 using a Schlenk filter, and dried on a vacuum pump.

Kinetics Runs. For unlabeled **1**, a sample of 10 mg of **1** in dry $CDCl_3$ at a height of 5 cm in a 5-mm NMR tube was prepared. For **1**-d_3, the solid **1**-d_3 on the Schlenk filter was first rinsed with 2 mL of $CDCl_3$ then mixed with an additional 2 mL of $CDCl_3$ and the resulting saturated solution was collected. A sample of this solution was used to fill a 5-mm NMR tube to a height of 2.5 cm, then diluted with $CDCl_3$ to a height of 5 cm in the tube.

The side-by-side samples were analyzed periodically by ^{1}H NMR, using an NMR macro that is provided in a later section.

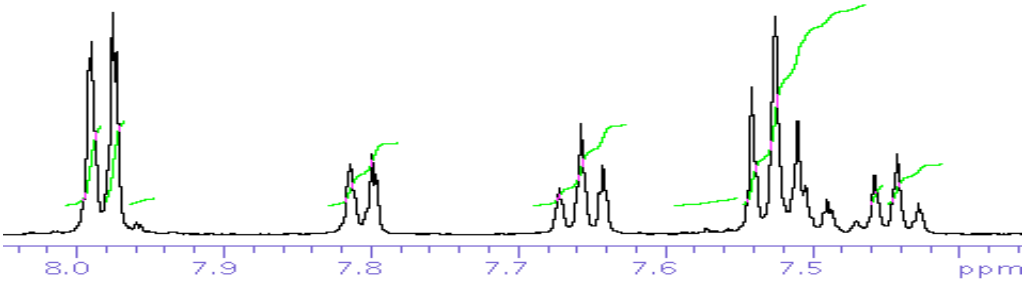
Analysis of Kinetics Data. While the unlabeled reaction could be followed in the ^{1}H NMR by looking at the CH_2 of the keto form of **1**, the CH of the enol **1'**, and the CH_3 of the acetophenone product, the labeled reaction could only be followed using changes in the aromatic protons, so analysis of the aromatic region was used for both unlabeled and labeled **1**. The other peaks served as a check in the unlabeled case. The aromatic region of the ^{1}H NMR exhibits some overlap of important peaks. Figure S1 shows the evolution of peaks versus time. The integration ranges were cut as shown and assigned as follows from left to right: half of **1** ortho Hs, overlap of half of **1** ortho Hs and half of acetophenone ortho Hs, half of acetophenone ortho Hs, enol **1'** ortho Hs, para H on **1**, para H on acetophenone, an overlapping set of peaks, and enol **1'** meta protons.

The integrations of these peaks for each labeled and unlabeled sample in sets of independent runs were collected in an Excel spreadsheet and the relative amount of each material was calculated at each time. Since the measurement depended on the integration of a single peak ("half") of doublets, and since the two peaks of the doublets involved are not equal in integration due to leaning, allowance was made in the calculation based on the relative integration of the peaks in pure samples. The limitations in the data derived from overlapping peaks provide uncertainty in the individual data points, and this added uncertainty to the ultimate isotope effect derived.

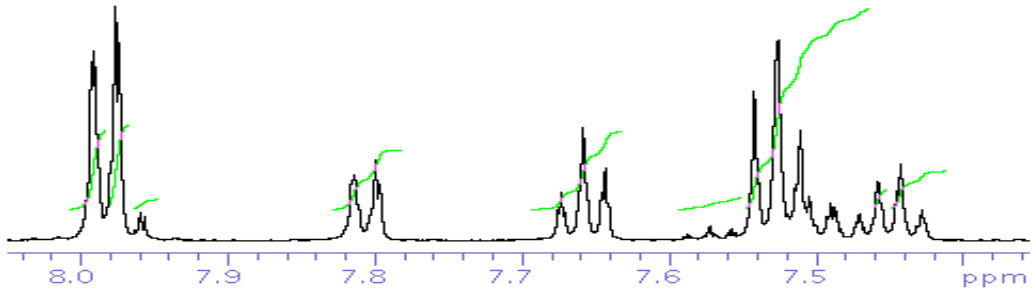
The relative amounts of the materials were then simulated on an Excel spreadsheet by numerical integration of an assumed first-order decay of **1**. It was assumed in the simulation that enol **1'** was in rapid equilibrium with **1** and that the ratio of **1** : **1'** did not change; the NMR data was consistent with these assumptions within the uncertainty of the measurements. Figure

Figure S1. Example ^{1}H NMR spectra of kinetics points for **1**.

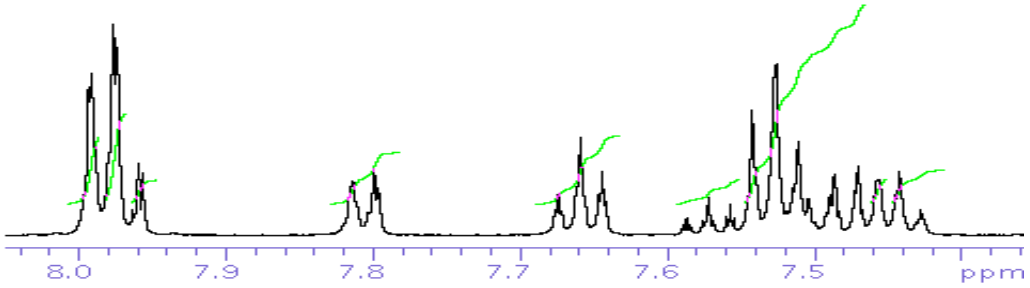
time = 0



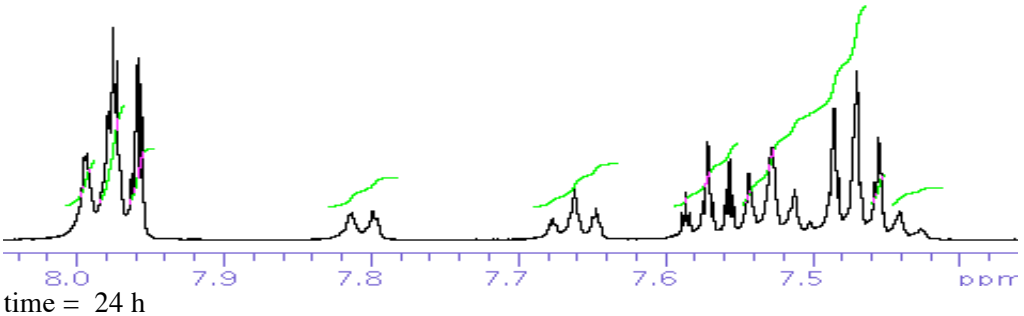
time = 1 h



time = 4 h



time = 12 h



time = 24 h

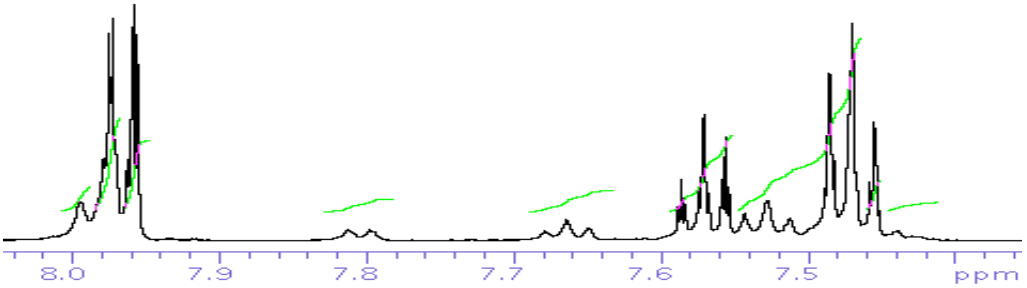
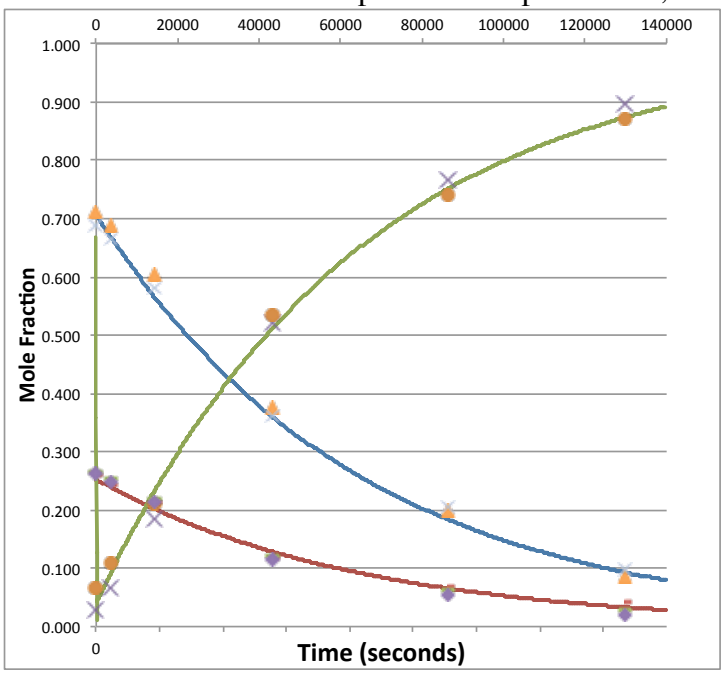


Figure S2. Example simulation for kinetics runs. The solid lines are calculated based on the numerical integration of first-order decay of **1**, with green for acetophenone, blue for **1**, and red for enol **1'**. The individual points are experimental, based on particular NMR integrations.



Computational Procedures and Supporting Computational Results

General

Calculations of structures, energies, and frequencies employed default procedures in Gaussian09[1,2,3] unless otherwise noted, except that in DFT calculations an ultrafine grid was usually employed. Complete structures and energetics are provided in sections below. All absolute energies are in Hartrees. All relative energies are presented in kcal/mol.

The program suite PROGDYN used for dynamics is a series of component programs written as either Unix shell scripts or awk programs. Gaussian09 was used to calculate the forces at each point in trajectories. A complete listing of the version of PROGDYN used here has been previously published (Nieves-Quinones, Y.; Singleton, D. A. *J. Am. Chem. Soc.* **2016**, *138*, 15167–15176), and a later section provides the configuration file and helper programs for data extraction. The latest version of this program can be obtained by emailing Daniel Singleton at singleton@chem.tamu.edu. The original version of this program was published in the Supporting Information of a previous paper.[4]

Initialization of Trajectories and Additional Details on Trajectories

The trajectories were in all cases quasiclassical. For quasiclassical trajectories, each normal mode in the transition structure of interest was given its zero-point energy plus a Boltzmann distribution of quantized vibrational energies. The desired energy in each of the

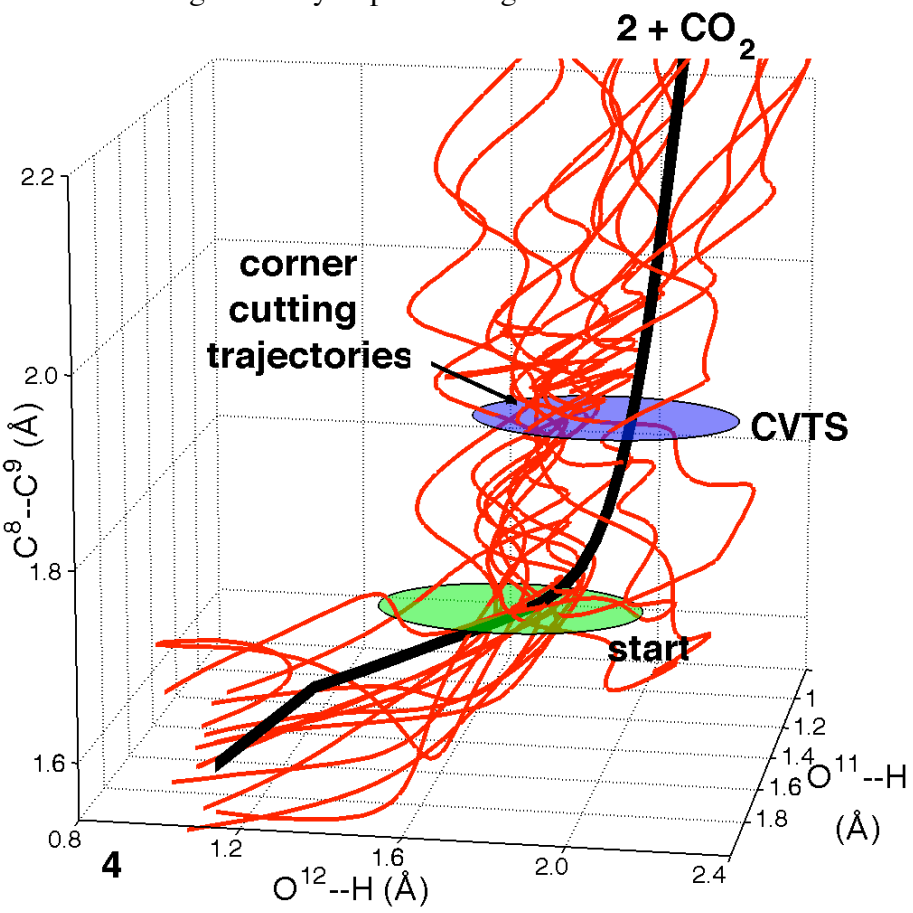
normal modes of the transition structure was mapped from a random number generator to a Boltzmann distribution set at 25 °C. The phase of each of the normal modes was mapped from a Gaussian distribution of random numbers. This distribution is not correct for a classical oscillator but it approximates that for a quantum oscillator in its ground state (only ignoring mode displacements outside of the classical limit), and it has the advantage that a larger portion of the trajectories start with an energy approximating the initially desired energy. The sign on the velocity of the normal modes was randomized. After an energy/force calculation on the initial geometry, the total initial energy was calculated and the trajectory was thrown out if the energy did not agree satisfactorily (within 1 kcal/mol) with the desired energy. (This is a variation of the conventional practice of scaling energies.[5]) The mode corresponding to the transition vector was treated classically. A sample PROGDYN parameter file (progdyn.conf) is given in a later section.

Trajectories were monitored with regard to the conservation of energy, and all did so within the limitations of the Verlet algorithm employed in PROGDYN.

"Corner Cutting" in Trajectories Initialized on the Reactant Side

The main text discusses the "corner cutting" of trajectories initialized from a point 0.5 bohr past the CVTS, toward the products. Here we show the results of trajectories started from 1.5 bohr before the CVTS, toward the reactants. Out of 161 trajectories started in this area, only 13 were productive, with the rest simply passing from reactant structure to reactant structure. Figure S3 below shows the paths of the productive trajectories. Because of where these trajectories were started, centered on the IRC in the middle of its "elbow", the trajectories do not have the opportunity to show the extreme corner-cutting seen in the trajectories started from the product side of the CVTS. However, the limited trajectories obtained show clearly the anharmonicity effect described in the main text, in that the trajectories are strongly biased toward passing on the "inside" portion of the CVTS. This is consistent with the contentions in the main text that a substantial portion of the trajectories combine both C-C and O-H motion as they pass the transition state and that anharmonicity in the transition state can be leading to errors in the KIE predictions.

Figure S3. The paths of productive trajectories started from a position 1.5 bohr before the CVTS. This figure shows all 13 of the productive trajectories obtained, and the key observation is that the trajectories show a strong tendancy to pass through the CVTS on its "inside".



Programs for Calculations

Program Suite PROGDYN

A complete listing of the subprograms for PROGDYN was provided in: Nieves-Quinones, Y.; Singleton, D. A. *J. Am. Chem. Soc.* **2016**, *138*, 15167–15176. Here, we just provide the configuration file for the trajectories (*progdyn.conf*), the program that collects the raw data (*proganal*) in the output file *dynfollowfile*, and some helper programs that were used to analyze the data from the trajectory calculations. A complete description of the use of these programs in context can be found in the SI for the reference above.

Here is a description of the helper programs used for the current study.

progcount – an awk program that counts the outcomes of the trajectories and keeps track of their time

progmatlistR – an awk program that pulls data out of dynfollowfile in a format suitable for use in Matlab.

hannah3d11comp.m - This is the Matlab version 2012 code that was used to generate Figure 4a. The date in this code was extracted using progmatlistR.

Program proganal

```
BEGIN {
nmrset=0
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

firsttitle=1
getline < "isomernumber"
isomer=$1
}
/ decarboxylation/ {
  if (firsttitle==1) {
    titlestring=$1" " $2" " $3" " $4" " $6" " $7" " $8
    printf("%s %s %s %s %s %s %s  ",$1,$2,$3,$4,$6,$7,$8)
    runpoint=$6
    }
  firsttitle++
  }
/Standard orientation/,/Rotational constants/ {
  if (($1>.5) && ($1<30)) {
    A[$1]=$4;B[$1]=$5;C[$1]=$6
    }
  }
END {
CC=Distance(9,8)
HOf=Distance(11,18)
HOi=Distance(12,18)
printf("%s %.3f %s %.3f %s %.3f ","CC",CC,"HOf",HOf,"HOi",HOi)
  if ((CC>2.3) && (OHf<1.0)) {
```

```
      print "Formed decarboxylation product XXXX"
#     system("date > nogo")
      }
   if ((CC)<1.7 && (HOf)<1.1) {
      printf(" %s ","in zwitterion")
#     print "Reformed zwitterion XXXX"
      }
   if ((CC)<1.6 && (HOi)<1.0) {
      print "Reformed neutral starting material XXXX"
      }
   if (runpoint>500) {
      print "   Too many points.  XXXX"
#     system("date > nogo")
      }
   system("date '+%b:%d:%Y %T'")
   system("tail -1 Echeck | grep XXXX")
   #system("uptime > uptimelist")
   }

function Distance(Atom1,Atom2) {
  return sqrt((A[Atom1]-A[Atom2])^2 + (B[Atom1]-B[Atom2])^2 + (C[Atom1]-C[Atom2])^2)
}

function Angle(Atom1,Atom2,Atom3) {
   value=((-
Distance(Atom1,Atom3)^2+Distance(Atom1,Atom2)^2+Distance(Atom2,Atom3)^2)/(2*Distance(Atom1,Atom2)*Distance(Ato
m2,Atom3)))
   return acos(value)
}

function asin(x) { return (180/3.141592)*atan2(x, sqrt(1-x*x)) }

function acos(x) { return (180/3.141592)*atan2(sqrt(1-x*x), x) }

function atan(x) { return (180/3.141592)*atan2(x,1) }

function Dihedral(Atom1,Atom2,Atom3,Atom4) {
   B1x=A[Atom2]-A[Atom1]
   B1y=B[Atom2]-B[Atom1]
   B1z=C[Atom2]-C[Atom1]
   B2x=A[Atom3]-A[Atom2]
   B2y=B[Atom3]-B[Atom2]
   B2z=C[Atom3]-C[Atom2]
   B3x=A[Atom4]-A[Atom3]
   B3y=B[Atom4]-B[Atom3]
   B3z=C[Atom4]-C[Atom3]
   modB2=sqrt((B2x^2)+(B2y^2)+(B2z^2))
# yAx is x-coord. etc of modulus of B2 times B1
   yAx=modB2*(B1x)
   yAy=modB2*(B1y)
   yAz=modB2*(B1z)
# CP2 is the crossproduct of B2 and B3
   CP2x=(B2y*B3z)-(B2z*B3y)
   CP2y=(B2z*B3x)-(B2x*B3z)
   CP2z=(B2x*B3y)-(B2y*B3x)
   termY=((yAx*CP2x)+(yAy*CP2y)+(yAz*CP2z))
# CP is the crossproduct of B1 and B2
   CPx=(B1y*B2z)-(B1z*B2y)
   CPy=(B1z*B2x)-(B1x*B2z)
   CPz=(B1x*B2y)-(B1y*B2x)
   termX=((CPx*CP2x)+(CPy*CP2y)+(CPz*CP2z))
  dihed4=(180/3.141592)*atan2(termY,termX)
```

```
  return dihed4
}

function killdyn(isomer) {
   system("rm -f dyn")
}
```

progdyn.conf

```
#This is the configuration file for PROGDYN.  This file is read by progdynstarterHP and
# the awk programs proggenHP, prog1stpoint, prog2ndpoint, and progdynb.
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.
method M062X/6-311+G**
nonstandard 0
rotationmode 1
method2 restricted
charge 0
multiplicity 1
processors 3
memory 7gb
killcheck 1
diagnostics 0
title decarboxylation PhCOCH2CO2H 2XPSPCM 298dis2
initialdis 2
timestep 5E-16
scaling 1.0
temperature 298.15
method3 scrf=(pcm,Solvent=dichloromethane)
method4 iop(2/9=2000)
methodfile 0
numimag 1
searchdir positive
classical 0
keepevery 99999
highlevel 9999
etolerance 1
damping 1.000
reversetraj true
```

Program progcount

```
/XXX/ {
   oldfile=file
   file=$1
   oldrun=run
   run=$7
   oldres=res
   res=$14
   oldtime=time
   time=$5
   if ((oldfile==file) && (oldrun==run)) {
      if ((oldres=="Formed") && (res=="Reformed")) {
         countgood++
         totaltime=totaltime+time+oldtime
         print time+oldtime
         }
      if ((res=="Formed") && (oldres=="Reformed")) {
         countgood++
         totaltime=totaltime+time+oldtime
```

```
      print time+oldtime
      }
    if ((oldres=="Reformed") && (res=="Reformed")) countSMrec++
    if ((oldres=="Formed") && (res=="Formed")) countProdrec++
    }
  }
END {
print "Productive runs",countgood
print "Recrossing to SM",countSMrec
print "Recrossing to Prod",countProdrec
print "averagetime",totaltime/(countgood*2)
}
```

Program progmatlistR

```
BEGIN {
  for (i=-502;i<502;i++) CC[i]=0
  oldisomer=0
  sign=-1
  list=14
}
/XXX/ {
oldres=res
res=$14
color="x"
if ((res=="Formed") && (oldres=="Reformed")) color="r"
if ((oldres=="Formed") && (res=="Reformed")) color="r"
if ((res=="Formed") && (oldres=="Formed")) color="b"
if ((res=="Reformed") && (oldres=="Reformed")) color="g"
}
/run/ {
if ($5==1) {
  oldisomer=runisomer
  runisomer=$7
  if (runisomer==oldisomer) sign=1
  if (runisomer>oldisomer) {
    sign=-1
    if ((CC[2]>0) && (color=="b")) {
      print "%",FILENAME,oldisomer,color
      mincc=10
      list++
      printf("%s%i%s"," x",list," = [")
      for (i=-502;i<502;i++) {
        if (CC[i]<2.3) {
          if (CC[i]>0) printf("%.3f",HOf[i])
          if ((CC[i]>0) && (CC[i+1]>0)) printf("%s",",")
          if (i==0) printf("%s",",")
          }
        }
      print "];"
      printf("%s%i%s"," y",list," = [")
      for (i=-502;i<502;i++) {
        if (CC[i]<2.3) {
          if (CC[i]>0) printf("%.3f",HOi[i])
          if ((CC[i]>0) && (CC[i+1]>0)) printf("%s",",")
          if (i==0) printf("%s",",")
          }
        }
      print "];"
      printf("%s%i%s"," z",list," = [")
      for (i=-502;i<502;i++) {
```

```
          if (CC[i]<2.3) {
            if (CC[i]>0) printf("%.3f",CC[i])
            if ((CC[i]<mincc) && (CC[i]>0)) mincc=CC[i]
            if ((CC[i]>0) && (CC[i+1]>0)) printf("%s",",")
            if (i==0) printf("%s",",")
            }
          }
        print "];"
        print "mincc",mincc
        }
      for (i=-502;i<502;i++) CC[i]=0
      }
    if (runisomer<oldisomer) {
      sign=-1
      for (i=-502;i<502;i++) CC[i]=0
      }
    }
pt=sign*$5
if ($8=="CC") {
  CC[pt]=$9
  HOf[pt]=$11
  HOi[pt]=$13
  }
if ($7=="CC") {
  CC[pt]=$8
  HOf[pt]=$10
  HOi[pt]=$12
  }
}
```

Matlab program hannah3d11comp.m

```
% n610/dynfollowfile 1
 x1 =
[0.901,0.922,0.948,0.977,1.005,1.028,1.044,1.052,1.052,1.043,1.027,1.004,0.977,0.948,0.923,0.903,0.895,0.898,0.914,0.937,0.966,0.995,1.020,1
.041,1.054,1.059,1.056,1.044,1.025,1.000,0.972,0.944,0.920,0.904,0.900,0.907,0.925,0.951,0.981,1.010,1.036,1.057,1.072,1.079,1.078,1.070,1.0
56,1.035,1.011,0.985,0.959,0.938,0.923,0.918,0.923,0.938,0.960,0.986,1.014,1.041,1.065,1.084,1.098,1.105,1.106,1.100,1.088,1.069,1.044,1.014
,0.983,0.951,0.924,0.905,0.898,0.904,0.921,0.948,0.979,1.010,1.040,1.065,1.083,1.095,1.100,1.098,1.088,1.072,1.050,1.023,0.993,0.964,0.937,0.
917,0.907,0.909,0.922,0.944,0.972,1.002,1.031,1.056,1.076,1.089,1.095,1.093,1.084,1.067,1.043,1.014,1.014,0.983,0.951,0.923,0.904,0.896,0.90
1,0.918,0.944,0.973,1.002,1.027,1.047,1.059,1.063,1.058,1.046,1.026,1.001,0.973,0.945,0.923,0.908,0.905,0.914,0.934,0.960,0.989,1.019,1.044,
1.064,1.078,1.084,1.082,1.073,1.056,1.034,1.007,0.979,0.952,0.929,0.916,0.913,0.922,0.942,0.967,0.996,1.025,1.051,1.071,1.086,1.093,1.092,1.
084,1.068,1.047,1.021,0.993,0.965,0.941,0.925,0.920,0.927,0.947,0.975,1.010,1.049,1.090,1.132,1.175,1.218,1.263,1.311,1.362,1.417,1.476,1.53
9,1.602];
 y1 =
[2.184,2.177,2.169,2.161,2.154,2.148,2.144,2.141,2.140,2.141,2.144,2.148,2.154,2.160,2.166,2.171,2.173,2.171,2.167,2.161,2.153,2.146,2.139,2
.133,2.128,2.125,2.122,2.120,2.118,2.118,2.117,2.115,2.111,2.104,2.090,2.071,2.046,2.017,1.986,1.955,1.925,1.899,1.876,1.858,1.845,1.837,1.8
34,1.837,1.844,1.854,1.865,1.876,1.882,1.883,1.878,1.866,1.849,1.831,1.813,1.797,1.784,1.775,1.770,1.769,1.773,1.781,1.793,1.808,1.826,1.847
,1.870,1.891,1.909,1.920,1.922,1.915,1.899,1.876,1.849,1.822,1.797,1.775,1.757,1.745,1.738,1.736,1.740,1.750,1.765,1.785,1.808,1.832,1.855,1.
875,1.888,1.893,1.890,1.882,1.872,1.862,1.854,1.850,1.851,1.857,1.868,1.885,1.906,1.931,1.960,1.992,1.992,2.025,2.059,2.091,2.118,2.140,2.15
5,2.164,2.169,2.171,2.172,2.171,2.171,2.170,2.169,2.168,2.167,2.166,2.165,2.164,2.161,2.156,2.148,2.134,2.116,2.094,2.069,2.043,2.019,1.998,
1.979,1.965,1.955,1.948,1.946,1.949,1.954,1.963,1.974,1.985,1.995,2.001,2.003,2.000,1.993,1.983,1.972,1.961,1.950,1.941,1.932,1.923,1.916,1.
908,1.900,1.892,1.884,1.875,1.864,1.850,1.831,1.805,1.771,1.729,1.682,1.632,1.579,1.526,1.473,1.420,1.367,1.314,1.258,1.200,1.137,1.071,1.00
1,0.933];
 z1 =
[2.283,2.266,2.250,2.235,2.219,2.205,2.191,2.177,2.164,2.152,2.140,2.128,2.118,2.108,2.098,2.089,2.080,2.072,2.064,2.056,2.048,2.040,2.032,2
.025,2.018,2.011,2.005,1.999,1.994,1.989,1.984,1.980,1.976,1.973,1.970,1.967,1.964,1.962,1.958,1.955,1.951,1.946,1.941,1.935,1.929,1.923,1.9
18,1.912,1.907,1.902,1.898,1.894,1.891,1.888,1.885,1.883,1.881,1.879,1.877,1.876,1.874,1.871,1.869,1.866,1.863,1.860,1.856,1.853,1.850,1.846
,1.843,1.840,1.837,1.835,1.832,1.830,1.829,1.827,1.826,1.824,1.823,1.821,1.819,1.816,1.813,1.810,1.807,1.803,1.800,1.797,1.795,1.792,1.790,1.
789,1.788,1.788,1.788,1.788,1.789,1.789,1.791,1.792,1.793,1.794,1.794,1.794,1.794,1.793,1.793,1.792,1.792,1.791,1.791,1.791,1.790,1.790,1.79
1,1.791,1.791,1.792,1.792,1.792,1.792,1.792,1.791,1.790,1.788,1.785,1.782,1.778,1.774,1.769,1.764,1.759,1.754,1.749,1.744,1.738,1.733,1.728,
1.724,1.719,1.714,1.709,1.704,1.699,1.694,1.688,1.681,1.674,1.666,1.658,1.650,1.641,1.634,1.626,1.619,1.613,1.607,1.602,1.598,1.594,1.591,1.
589,1.587,1.586,1.585,1.584,1.583,1.581,1.579,1.577,1.575,1.574,1.572,1.572,1.571,1.572,1.572,1.574,1.576,1.578,1.581,1.584,1.587,1.590,1.59
3,1.596];
% n610/dynfollowfile 2
 x2 =
```

```
[1.049,1.025,0.994,0.960,0.928,0.901,0.885,0.884,0.897,0.923,0.955,0.989,1.022,1.049,1.069,1.081,1.084,1.078,1.063,1.040,1.011,0.977,0.943,0
.913,0.892,0.884,0.891,0.912,0.942,0.976,1.011,1.042,1.068,1.086,1.096,1.098,1.092,1.077,1.055,1.028,0.996,0.963,0.932,0.908,0.895,0.896,0.9
10,0.935,0.966,0.999,1.030,1.057,1.078,1.090,1.095,1.091,1.078,1.058,1.031,0.999,0.965,0.934,0.934,0.908,0.894,0.893,0.907,0.932,0.963,0.997
,1.029,1.057,1.078,1.091,1.095,1.091,1.078,1.057,1.030,0.997,0.962,0.930,0.904,0.890,0.890,0.905,0.932,0.966,1.002,1.037,1.068,1.094,1.112,1.
124,1.128,1.125,1.115,1.099,1.078,1.052,1.023,0.994,0.967,0.945,0.932,0.928,0.935,0.952,0.976,1.005,1.036,1.066,1.095,1.120,1.143,1.161,1.17
6,1.186,1.193,1.196,1.196,1.192,1.185,1.174,1.161,1.145,1.126,1.105,1.082,1.059,1.035,1.013,0.994,0.979,0.970,0.968,0.973,0.985,1.001,1.021,
1.042,1.061,1.078,1.091,1.099,1.101,1.096,1.085,1.067,1.044,1.015,0.985,0.954,0.927,0.908,0.901,0.906,0.922,0.948,0.979,1.011,1.042,1.070,1.
093,1.111,1.125,1.134,1.139,1.141,1.141,1.140,1.138,1.137,1.137,1.140,1.145,1.155,1.168,1.185,1.206,1.232,1.262,1.295,1.331,1.369,1.406,1.44
1];
 y2 =
[1.842,1.845,1.852,1.862,1.873,1.882,1.885,1.881,1.868,1.849,1.826,1.802,1.781,1.763,1.750,1.743,1.741,1.744,1.754,1.768,1.788,1.810,1.833,1
.855,1.870,1.877,1.873,1.860,1.841,1.819,1.798,1.779,1.764,1.754,1.749,1.749,1.754,1.763,1.778,1.796,1.818,1.841,1.863,1.881,1.892,1.894,1.8
88,1.877,1.862,1.846,1.832,1.821,1.814,1.811,1.811,1.815,1.823,1.834,1.848,1.864,1.881,1.898,1.898,1.911,1.919,1.919,1.912,1.899,1.884,1.868
,1.853,1.841,1.831,1.825,1.823,1.824,1.828,1.836,1.847,1.860,1.875,1.889,1.901,1.906,1.903,1.892,1.875,1.854,1.833,1.813,1.796,1.782,1.771,1.
765,1.761,1.761,1.765,1.771,1.781,1.793,1.808,1.823,1.838,1.850,1.857,1.857,1.850,1.836,1.817,1.795,1.771,1.747,1.724,1.703,1.684,1.666,1.65
1,1.638,1.626,1.617,1.610,1.606,1.604,1.605,1.608,1.615,1.625,1.637,1.652,1.669,1.687,1.705,1.723,1.739,1.752,1.761,1.768,1.771,1.773,1.774,
1.775,1.777,1.780,1.784,1.789,1.794,1.800,1.806,1.812,1.818,1.824,1.830,1.834,1.834,1.830,1.818,1.799,1.772,1.739,1.703,1.665,1.626,1.588,1.
551,1.515,1.482,1.449,1.419,1.390,1.363,1.338,1.314,1.292,1.272,1.252,1.232,1.213,1.192,1.170,1.146,1.119,1.091,1.060,1.027,0.994,0.964,0.93
8];
 z2 =
[2.289,2.273,2.258,2.243,2.229,2.215,2.202,2.190,2.178,2.167,2.156,2.147,2.138,2.129,2.121,2.114,2.106,2.099,2.092,2.086,2.079,2.072,2.065,2
.057,2.050,2.043,2.036,2.028,2.022,2.015,2.008,2.002,1.995,1.989,1.983,1.977,1.971,1.964,1.958,1.952,1.946,1.940,1.934,1.927,1.921,1.915,1.9
09,1.903,1.897,1.891,1.886,1.880,1.875,1.869,1.863,1.857,1.851,1.845,1.839,1.832,1.825,1.819,1.819,1.812,1.806,1.799,1.794,1.788,1.783,1.778
,1.773,1.768,1.764,1.759,1.755,1.751,1.747,1.743,1.739,1.735,1.731,1.728,1.724,1.722,1.719,1.717,1.715,1.713,1.712,1.710,1.709,1.707,1.706,1.
704,1.702,1.700,1.698,1.695,1.693,1.690,1.687,1.684,1.681,1.678,1.675,1.671,1.668,1.664,1.660,1.656,1.650,1.645,1.639,1.633,1.627,1.621,1.61
5,1.609,1.603,1.597,1.591,1.586,1.581,1.576,1.572,1.568,1.565,1.562,1.560,1.558,1.557,1.557,1.556,1.557,1.558,1.559,1.561,1.563,1.566,1.569,
1.572,1.576,1.579,1.582,1.585,1.588,1.591,1.593,1.596,1.599,1.602,1.606,1.609,1.612,1.616,1.620,1.624,1.629,1.634,1.639,1.643,1.648,1.652,1.
657,1.660,1.664,1.667,1.669,1.671,1.673,1.674,1.675,1.675,1.675,1.674,1.673,1.671,1.667,1.663,1.658,1.652,1.644,1.636,1.626,1.615,1.603,1.59
0];
% n610/dynfollowfile 4
 x3 =
[1.496,1.450,1.405,1.361,1.321,1.283,1.248,1.214,1.182,1.151,1.122,1.093,1.067,1.043,1.022,1.006,0.995,0.990,0.991,0.998,1.010,1.025,1.043,1
.062,1.080,1.097,1.111,1.123,1.130,1.133,1.132,1.125,1.114,1.097,1.076,1.051,1.023,0.994,0.966,0.943,0.926,0.919,0.922,0.935,0.956,0.982,1.0
10,1.036,1.060,1.079,1.093,1.101,1.103,1.100,1.090,1.076,1.057,1.035,1.011,0.987,0.965,0.948,0.938,0.937,0.944,0.959,0.980,1.004,1.029,1.053
,1.074,1.092,1.105,1.113,1.115,1.111,1.102,1.087,1.066,1.040,1.011,0.981,0.952,0.928,0.913,0.908,0.916,0.934,0.959,0.987,1.016,1.041,1.062,1.
076,1.083,1.082,1.073,1.057,1.035,1.007,0.978,0.948,0.924,0.907,0.902,0.909,0.927,0.953,0.982,1.011,1.037,1.058,1.071,1.077,1.074,1.063,1.04
4,1.019,0.989,0.958,0.929,0.907,0.895,0.896,0.910,0.934,0.964,0.995,1.024,1.048,1.064,1.073,1.073,1.064,1.047,1.023,0.994,0.963,0.933,0.909,
0.895,0.895,0.907,0.930,0.961,0.994,1.026,1.054,1.077,1.093,1.101,1.102,1.095,1.080,1.059,1.032,1.032,1.001,0.968,0.938,0.914,0.899,0.898,0.
909,0.931,0.960,0.992,1.023,1.051,1.073,1.088,1.097,1.097,1.090,1.076,1.055,1.029,0.999,0.968,0.939,0.917,0.904,0.904,0.916,0.938,0.967,1.00
0,1.032,1.061,1.087,1.107,1.123,1.133,1.138,1.137,1.133,1.124,1.112,1.096,1.078,1.058,1.038,1.018,0.999,0.984,0.973,0.967,0.967,0.973,0.984,
0.999,1.016,1.035,1.054,1.072,1.088,1.101,1.111,1.118,1.120,1.119,1.114,1.104,1.092,1.076,1.057,1.037,1.018,0.999,0.983,0.972,0.967,0.969,0.
979,0.994,1.016,1.043,1.073,1.107,1.144,1.184,1.228,1.276,1.328,1.385,1.445];
 y3 =
[0.955,1.009,1.063,1.114,1.161,1.204,1.243,1.279,1.312,1.343,1.373,1.401,1.428,1.454,1.477,1.498,1.515,1.528,1.538,1.544,1.548,1.549,1.550,1
.550,1.551,1.553,1.555,1.559,1.565,1.572,1.580,1.590,1.602,1.616,1.632,1.650,1.670,1.690,1.711,1.729,1.743,1.751,1.752,1.747,1.736,1.723,1.7
08,1.694,1.682,1.672,1.664,1.660,1.658,1.660,1.665,1.674,1.686,1.700,1.717,1.735,1.753,1.767,1.778,1.783,1.783,1.777,1.768,1.758,1.748,1.740
,1.734,1.731,1.732,1.737,1.746,1.759,1.775,1.796,1.820,1.847,1.877,1.908,1.938,1.965,1.986,2.001,2.007,2.008,2.004,1.998,1.992,1.987,1.983,1.
983,1.985,1.990,1.997,2.007,2.019,2.033,2.049,2.064,2.076,2.085,2.087,2.083,2.073,2.059,2.044,2.029,2.016,2.006,2.000,1.997,1.999,2.004,2.01
3,2.026,2.041,2.057,2.074,2.087,2.095,2.098,2.094,2.086,2.075,2.063,2.052,2.043,2.035,2.030,2.026,2.025,2.026,2.028,2.031,2.035,2.038,2.037,
2.032,2.019,2.000,1.975,1.946,1.916,1.886,1.859,1.835,1.814,1.798,1.787,1.780,1.778,1.781,1.788,1.788,1.800,1.814,1.828,1.840,1.846,1.844,1.
834,1.817,1.796,1.775,1.756,1.740,1.728,1.721,1.719,1.722,1.728,1.739,1.754,1.771,1.790,1.810,1.828,1.841,1.847,1.844,1.833,1.813,1.789,1.76
2,1.734,1.708,1.684,1.662,1.642,1.626,1.612,1.601,1.594,1.589,1.587,1.588,1.592,1.598,1.605,1.614,1.622,1.629,1.633,1.634,1.630,1.623,1.612,
1.598,1.583,1.568,1.553,1.540,1.528,1.518,1.510,1.503,1.499,1.495,1.493,1.493,1.494,1.496,1.499,1.502,1.505,1.508,1.508,1.506,1.499,1.487,1.
470,1.448,1.421,1.392,1.359,1.324,1.286,1.246,1.202,1.155,1.104,1.049,0.992];
 z3 =
[1.543,1.547,1.551,1.554,1.557,1.560,1.562,1.564,1.566,1.567,1.568,1.568,1.569,1.569,1.570,1.571,1.573,1.575,1.577,1.581,1.584,1.588,1.592,1
.597,1.601,1.606,1.610,1.614,1.619,1.623,1.627,1.630,1.634,1.637,1.640,1.644,1.647,1.651,1.655,1.659,1.663,1.668,1.673,1.678,1.683,1.688,1.6
93,1.697,1.702,1.706,1.709,1.712,1.714,1.716,1.717,1.717,1.717,1.717,1.715,1.714,1.713,1.711,1.709,1.707,1.704,1.702,1.699,1.696,1.694,1.691
,1.689,1.686,1.684,1.682,1.681,1.680,1.679,1.678,1.678,1.679,1.680,1.682,1.685,1.688,1.693,1.697,1.703,1.709,1.715,1.721,1.728,1.735,1.741,1.
748,1.754,1.760,1.765,1.770,1.773,1.776,1.779,1.781,1.782,1.783,1.784,1.785,1.785,1.785,1.784,1.784,1.783,1.782,1.781,1.779,1.778,1.777,1.77
6,1.775,1.775,1.774,1.774,1.774,1.775,1.776,1.777,1.778,1.780,1.781,1.783,1.784,1.786,1.787,1.789,1.791,1.794,1.797,1.800,1.803,1.807,1.810,
1.814,1.817,1.821,1.824,1.827,1.829,1.831,1.832,1.833,1.833,1.833,1.832,1.832,1.831,1.830,1.829,1.829,1.829,1.829,1.829,1.829,1.829,1.830,1.
831,1.833,1.834,1.836,1.837,1.839,1.841,1.843,1.844,1.846,1.848,1.849,1.850,1.851,1.852,1.852,1.853,1.853,1.853,1.853,1.853,1.853,1.853,1.85
2,1.851,1.851,1.850,1.848,1.846,1.844,1.841,1.838,1.835,1.832,1.828,1.825,1.821,1.818,1.815,1.813,1.810,1.808,1.806,1.805,1.803,1.801,1.799,
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58,1.881,1.897,1.905,1.905,1.899,1.889,1.877,1.867,1.859,1.854,1.853,1.856,1.863,1.875,1.890,1.910,1.933,1.960,1.988,2.015,2.015,2.040,2.058
,2.070,2.075,2.074,2.072,2.069,2.068,2.071,2.076,2.084,2.096,2.110,2.127,2.147,2.168,2.191,2.213,2.233,2.250,2.262,2.269,2.271,2.271,2.269,2.
267,2.266,2.264,2.264,2.264,2.265,2.266,2.268,2.270,2.274,2.276,2.278,2.276,2.270,2.258,2.241,2.221,2.200,2.178,2.158,2.140,2.124,2.112,2.10
3,2.097,2.094,2.095,2.098,2.104,2.110,2.114,2.113,2.105,2.089,2.067,2.039,2.010,1.981,1.955,1.933,1.916,1.903,1.896,1.894,1.897,1.905,1.918,
1.936,1.956,1.979,2.000,2.018,2.029,2.032,2.026,2.014,1.997,1.980,1.963,1.948,1.935,1.927,1.921,1.920,1.922,1.927,1.936,1.948,1.961,1.975,1.
988,1.996,1.997,1.989,1.974,1.953,1.930,1.907,1.886,1.869,1.857,1.851,1.850,1.855,1.866,1.882,1.902,1.926,1.950,1.973,1.991,2.002,2.005,2.00
2,1.996,1.989,1.983,1.981,1.981,1.985,1.992,2.002,2.014,];
 z29 =
[2.293,2.279,2.265,2.252,2.239,2.226,2.213,2.201,2.189,2.177,2.166,2.155,2.144,2.134,2.125,2.116,2.107,2.098,2.090,2.081,2.073,2.064,2.056,2
.047,2.039,2.030,2.021,2.013,2.005,1.997,1.989,1.982,1.976,1.970,1.964,1.959,1.955,1.950,1.946,1.941,1.937,1.933,1.929,1.925,1.921,1.916,1.9
12,1.907,1.903,1.898,1.893,1.888,1.882,1.877,1.871,1.865,1.859,1.852,1.846,1.840,1.833,1.827,1.821,1.814,1.808,1.802,1.796,1.796,1.790,1.784
,1.778,1.772,1.765,1.758,1.752,1.745,1.738,1.732,1.725,1.719,1.713,1.707,1.701,1.696,1.690,1.684,1.678,1.672,1.666,1.659,1.652,1.645,1.638,1.
630,1.623,1.616,1.609,1.602,1.596,1.591,1.586,1.582,1.578,1.576,1.573,1.572,1.571,1.570,1.570,1.570,1.570,1.571,1.572,1.574,1.576,1.578,1.58
0,1.583,1.585,1.589,1.592,1.596,1.601,1.606,1.611,1.616,1.622,1.628,1.635,1.641,1.648,1.654,1.661,1.668,1.674,1.680,1.685,1.691,1.695,1.700,
1.704,1.708,1.713,1.718,1.723,1.729,1.735,1.741,1.748,1.755,1.762,1.769,1.777,1.784,1.792,1.800,1.809,1.817,1.826,1.834,1.843,1.853,1.862,1.
872,1.882,1.892,1.903,1.914,1.925,1.936,1.947,1.958,1.970,1.981,1.992,2.003,2.015,2.027,2.039,2.051,2.064,2.077,2.091,2.106,2.121,2.136,2.15
2,2.168,2.184,2.200,2.216,2.233,2.249,2.266,2.282,2.299,];
% n616/dynfollowfile 2
 x30 =
[0.932,0.954,0.978,1.002,1.022,1.037,1.046,1.047,1.042,1.030,1.013,0.991,0.967,0.944,0.925,0.912,0.909,0.915,0.929,0.950,0.973,0.996,1.016,1
.031,1.040,1.043,1.039,1.029,1.014,0.995,0.974,0.955,0.938,0.928,0.926,0.933,0.947,0.967,0.991,1.017,1.041,1.064,1.083,1.098,1.109,1.115,1.1
16,1.111,1.102,1.087,1.068,1.044,1.016,0.987,0.959,0.934,0.916,0.908,0.911,0.925,0.947,0.974,1.002,1.027,1.049,1.065,1.073,1.074,1.067,1.053
,1.032,1.006,0.977,0.977,0.948,0.923,0.906,0.900,0.905,0.922,0.947,0.975,1.003,1.028,1.048,1.061,1.065,1.062,1.050,1.032,1.007,0.979,0.951,0.
```

```
925,0.906,0.898,0.902,0.918,0.942,0.970,0.999,1.025,1.047,1.061,1.068,1.067,1.058,1.043,1.022,0.996,0.970,0.945,0.926,0.915,0.915,0.926,0.94
6,0.972,1.002,1.031,1.060,1.084,1.105,1.122,1.134,1.142,1.145,1.144,1.140,1.131,1.120,1.107,1.091,1.073,1.056,1.038,1.021,1.007,0.996,0.989,
0.987,0.990,0.998,1.010,1.026,1.044,1.065,1.087,1.109,1.132,1.156,1.180,1.205,1.231,1.259,1.289,1.322,1.358,1.396,1.437,1.478];
 y30 =
[1.896,1.876,1.857,1.839,1.826,1.817,1.813,1.816,1.823,1.836,1.852,1.871,1.892,1.912,1.929,1.941,1.947,1.947,1.940,1.928,1.914,1.899,1.885,1
.871,1.860,1.850,1.843,1.838,1.834,1.832,1.831,1.829,1.824,1.816,1.802,1.782,1.758,1.730,1.700,1.671,1.643,1.618,1.596,1.579,1.567,1.559,1.5
56,1.558,1.565,1.577,1.594,1.615,1.640,1.668,1.696,1.723,1.746,1.764,1.774,1.779,1.780,1.779,1.780,1.782,1.788,1.797,1.810,1.826,1.845,1.866
,1.890,1.916,1.943,1.943,1.969,1.994,2.015,2.031,2.043,2.049,2.053,2.055,2.056,2.057,2.059,2.062,2.066,2.071,2.076,2.083,2.091,2.099,2.106,2.
113,2.116,2.115,2.108,2.097,2.082,2.064,2.046,2.027,2.011,1.995,1.982,1.972,1.964,1.958,1.956,1.955,1.955,1.954,1.951,1.944,1.930,1.910,1.88
5,1.856,1.825,1.795,1.766,1.739,1.715,1.694,1.675,1.659,1.645,1.634,1.624,1.617,1.612,1.609,1.607,1.607,1.607,1.608,1.608,1.607,1.604,1.598,
1.588,1.574,1.557,1.536,1.512,1.486,1.459,1.431,1.402,1.373,1.344,1.315,1.284,1.253,1.220,1.185,1.148,1.108,1.066,1.023,0.980];
 z30 =
[2.295,2.279,2.263,2.248,2.233,2.218,2.203,2.188,2.174,2.161,2.148,2.135,2.123,2.112,2.101,2.091,2.081,2.072,2.064,2.057,2.050,2.044,2.039,2
.033,2.028,2.023,2.018,2.013,2.007,2.002,1.997,1.992,1.987,1.983,1.979,1.976,1.973,1.971,1.969,1.967,1.965,1.963,1.962,1.960,1.957,1.955,1.9
51,1.947,1.943,1.937,1.932,1.926,1.921,1.915,1.910,1.905,1.900,1.896,1.892,1.888,1.885,1.882,1.880,1.878,1.875,1.873,1.871,1.869,1.866,1.863
,1.860,1.856,1.853,1.853,1.849,1.846,1.842,1.839,1.836,1.832,1.829,1.826,1.823,1.819,1.816,1.812,1.809,1.805,1.801,1.797,1.792,1.787,1.782,1.
777,1.771,1.766,1.760,1.755,1.750,1.746,1.741,1.737,1.734,1.730,1.727,1.724,1.722,1.719,1.716,1.713,1.710,1.706,1.702,1.697,1.692,1.686,1.68
1,1.674,1.668,1.661,1.655,1.648,1.641,1.635,1.628,1.622,1.615,1.609,1.603,1.597,1.591,1.585,1.579,1.573,1.566,1.560,1.554,1.548,1.542,1.537,
1.533,1.529,1.527,1.525,1.525,1.525,1.525,1.526,1.528,1.531,1.534,1.538,1.541,1.545,1.548,1.551,1.553,1.554,1.555,1.556,1.556,1.556];

 y100=
[1.023,1.198,1.301,1.396,1.477,1.546,1.611,1.672,1.729,1.783,1.830,1.868,1.900,1.925,1.947,1.966,1.982,1.997,2.010,2.023,2.035,2.047,2.058,2
.070,2.082,2.093,2.104]
 x100=
[1.603,1.301,1.211,1.140,1.094,1.064,1.043,1.027,1.015,1.006,0.999,0.994,0.990,0.987,0.984,0.981,0.979,0.977,0.975,0.974,0.972,0.971,0.970,0
.970,0.969,0.968,0.968]
 z100=
[1.535,1.575,1.581,1.589,1.598,1.606,1.615,1.625,1.636,1.652,1.675,1.705,1.740,1.778,1.817,1.857,1.898,1.939,1.979,2.020,2.062,2.103,2.144,2
.184,2.225,2.266,2.307]

%% - old code example for reading from excel spreadsheet
%x1 = xlsread('~/spindata.xlsx',1,'B2:B550','basic');
%y1 = xlsread('~/spindata.xlsx',1,'C2:C550','basic');
%z1 = xlsread('~/spindata.xlsx',1,'D2:D550','basic');

figure(2216)
hFig = figure(2216);
set(gca, 'LooseInset', get(gca,'TightInset'))
set(hFig, 'Position', [1 1 1056 1092],'color',[1 1 1])
plot3(x1,y1,z1,'r','LineWidth',4)
hold on
plot3(x2,y2,z2,'r','LineWidth',4)
hold on
%plot3(x3,y3,z3,'g','LineWidth',4)
hold on
%plot3(x4,y4,z4,'b','LineWidth',4)
hold on
plot3(x5,y5,z5,'r','LineWidth',4)
hold on
plot3(x6,y6,z6,'r','LineWidth',4)
hold on
plot3(x7,y7,z7,'r','LineWidth',4)
hold on
plot3(x8,y8,z8,'r','LineWidth',4)
hold on
%plot3(x9,y9,z9,'g','LineWidth',4)
hold on
plot3(x10,y10,z10,'r','LineWidth',4)
hold on
plot3(x11,y11,z11,'r','LineWidth',4)
hold on
%plot3(x12,y12,z12,'b','LineWidth',4)
hold on
plot3(x13,y13,z13,'r','LineWidth',4)
hold on
```

```
plot3(x14,y14,z14,'r','LineWidth',4)
hold on
%plot3(x15,y15,z15,'g','LineWidth',4)
hold on
plot3(x16,y16,z16,'r','LineWidth',4)
hold on
plot3(x17,y17,z17,'r','LineWidth',4)
hold on
plot3(x18,y18,z18,'r','LineWidth',4)
hold on
plot3(x19,y19,z19,'r','LineWidth',4)
hold on
plot3(x20,y20,z20,'r','LineWidth',4)
hold on
plot3(x21,y21,z21,'r','LineWidth',4)
hold on
plot3(x22,y22,z22,'r','LineWidth',4)
hold on
plot3(x23,y23,z23,'r','LineWidth',4)
hold on
%plot3(x24,y24,z24,'b','LineWidth',4)
hold on
%plot3(x25,y25,z25,'b','LineWidth',4)
hold on
%plot3(x26,y26,z26,'g','LineWidth',4)
hold on
plot3(x27,y27,z27,'r','LineWidth',4)
hold on
%plot3(x28,y28,z28,'b','LineWidth',4)
hold on
%plot3(x29,y29,z29,'b','LineWidth',4)
hold on
plot3(x30,y30,z30,'r','LineWidth',4)
hold on
plot3(x100,y100,z100,'k','LineWidth',12)
hold on
[x y z]=sphere;
surf(.17*x+1.03,.4*y+1.80,.1*z+1.65,'facealpha',0.25,'edgealpha',0.25,'cdatamapping','direct')

view(8,12)
xlabel('O^{11}--H (\fontname{Geneva}≈\fontname{Helvetica})  ', 'FontSize', 36, 'fontname', 'Helvetica')
ylabel({'O^{12}--H';'(\fontname{Geneva}≈\fontname{Helvetica})'}, 'FontSize', 36, 'fontname',
'Helvetica','HorizontalAlignment','center')
zlabel('C^{8}--C^{9} (\fontname{Geneva}≈\fontname{Helvetica})', 'FontSize', 36, 'fontname', 'Helvetica')

%%set label positions
hxlabel = get(gca, 'XLabel');
set(hxlabel,'Position',[1.35, 0.75,1.52]);
hylabel = get(gca, 'YLabel');
set(hylabel,'Position',[1.69, 1.83,1.52]);
hzlabel = get(gca, 'ZLabel');
set(hzlabel,'Position',[0.775, 0.73, 1.9]);

annotation('textbox',[.55 0.565 0.23
0.05],'LineStyle','none','String',{'CVTS'},'FontSize',42,'fontweight','bold','FitBoxToText','off');
annotation('arrow',[0.545 0.505],[0.585 0.585],'LineWidth',4,'Color',[0 0 0],'HeadStyle','deltoid','HeadLength',15);
annotation('textbox',[0.27 0.916 0.23 0.05],'LineStyle','none','String',{'2 +
CO_{2}'},'FontSize',42,'fontweight','bold','FitBoxToText','off');
%annotation('arrow',[0.4308 0.36],...
%    [0.85 0.9],'LineWidth',4,'Color',[0 0 0],'HeadStyle','deltoid','HeadLength',15);
annotation('textbox',[0.752 0.049 0.23 0.05],'LineStyle','none','String',{'4'},'FontSize',42,'fontweight','bold','FitBoxToText','off');
annotation('textbox',[0.752 0.25 0.23 0.05],'LineStyle','none','String',{'IRC'},'FontSize',42,'fontweight','bold','FitBoxToText','off');
```

```
annotation('arrow',[0.77 0.74],[0.24 0.17],'LineWidth',4,'Color',[0 0 0],'HeadStyle','deltoid','HeadLength',15);
annotation('textbox',[.56 0.365 0.23 0.05],'LineStyle','none','String',{'6'},'FontSize',42,'fontweight','bold','FitBoxToText','off');
annotation('arrow',[0.555 0.515],[0.385 0.385],'LineWidth',4,'Color',[0 0 0],'HeadStyle','deltoid','HeadLength',15);

[x y z]=ellipse(0.18,0.50,3,[0.98,1.89,1.84]);
fill3(x,y,z,'b','linestyle','-','LineWidth',2,'facealpha',0.55);


grid on
axis('manual',[0.80,1.6,0.80,2.4,1.54,2.1])

set(gca,'XTick',[0.8 1.0 1.2 1.4 1.6],'xticklabel',{''},'TickLength',[0.01 0.01])
set(gca,'YTick',[0.8 1.2 1.6 2.0 2.4],'yticklabel',{''},'TickLength',[0.01 0.01])
set(gca,'zTick',[1.4 1.6 1.8 2.0 2.1],'zticklabel',{'','1.6','1.8','2.0',''},'TickLength',[0.01 0.01])
set(gca,'LineWidth',1.5)
set(gca,'FontSize',28)
set(gca,'PlotBoxAspectRatio',[1 1 1])
set(gca,'projection','perspective')
set(gca,'position',[.09 .1 .82 .87])
set(gca,'GridLineStyle',':')
ah(1)=gca;
ah(2)=axes('parent',gcf,'position',get(ah(1),'position'),'color','none','xlim',[0.80,1.6],...
   'ylim',[0.80,2.6],'zlim',[1.40,2.32],'PlotBoxAspectRatio',[1 1 1],'projection','perspective','view',[8 12],...
   'gridlinestyle','none','xgrid','off','ygrid','off',...
   'xtick',[0.82 1.0 1.22 1.42],'ytick',[.95 1.35 1.9 2.38],'ztick',[1.41],'TickLength',[0.00 0.00],'FontSize',28,...
   'xticklabel',{'0.8','1','1.2','1.4', ''},'yticklabel',{'0.8','1.2','1.6','2.0'},'zticklabel',{"","","","",""});
hlink=linkprop(ah,'view')
%set(gca,'CameraPosition',[-2.156 -2.345 6.272])
```

Sample Input Files for Gaussrate

The sample input files below are those used for the M06-2X/6-311+G**/PCM calculations. In the example shown, the esp.fu71, esp.fu73, and esp.fu75 files are not actually used for the calculation, but these files are shown because they were used in an initial crude calculation to establish the starting geometries. The starting geometries were then taken from the esp.fu61 output file for the crude calculation and put in the poly.fu5 file for the production calculation. To calculate isotope effects, the poly.fu5 file was modified in the top atom list to designate the isotope used. (There are multiple ways to calculate isotope effects in Gaussrate / Polyrate. This choice, rerunning the complete path with the isotope, is the most computationally intensive but the most straightforward.)

poly.fu5

```
*General

  TITLE
 decarboxylation of benzoylacetic acid
 END

 ATOMS
   1  C
   2  C
   3  C
   4  C
   5  C
   6  C
   7  C
   8  C
```

```
  9  C
 10  O
 11  O
 12  O
 13  H
 14  H
 15  H
 16  H
 17  H
 18  H
 19  H
 20  H
END

NOSUPERMOL

WRITEFU31 ON
INPUNIT AU

*OPTIMIZATION

OPTMIN  OHOOK
OPTTS   OHOOK

*SECOND

HESSCAL HHOOK

*REACT1
STATUS 2
SPECIES   NONLINRP
GEOM
  1        4.62791384      0.07687520      0.02241563
  2        2.33738022      0.01377705     -1.24836205
  3        0.06872079     -0.05179531      0.10802993
  4        0.11995548     -0.05839726      2.74925401
  5        2.41978841     -0.00185629      4.01679944
  6        4.66939016      0.06820241      2.65681398
  7       -2.33788159     -0.11718896     -1.33911593
  8       -4.80426015     -0.05189376      0.11915389
  9       -7.28497969      0.02753770     -1.34925313
 10        -9.26222839      0.19009603     -0.23916604
 11        -2.31671000     -0.22246254     -3.64256538
 12        -7.19658256     -0.10152530     -3.84823727
 13        -1.61232325     -0.11374995      3.83739986
 14         2.45395898     -0.01128398      6.06268678
 15         6.45954055      0.11677093      3.64949998
 16         6.38101365      0.13347414     -1.03192279
 17         2.27138897      0.01810009     -3.29361094
 18        -5.41820985     -0.19634164     -4.38710065
 19        -4.89647211     -1.71607585      1.34300252
 20        -4.81008606      1.57712960      1.38797249
END

*PROD1
STATUS 2
SPECIES   NONLINRP
GEOM
  1        3.22822139      1.20174946     -0.69295653
  2        1.05207209      0.02216390     -1.57978917
  3       -0.79507087     -0.81422249      0.11372774
  4       -0.40139535     -0.50228536      2.70788950
```

```
  5        1.77509269     0.67104953     3.58732545
  6        3.59257970     1.53574394     1.88951631
  7       -3.16249652    -1.95036066    -0.85966137
  8       -5.39331520    -1.82741000     0.31758962
  9       -3.79363304     3.92319291    -1.69684570
 10       -3.79451203     4.57760829     0.38540750
 11       -2.82485036    -3.06557866    -3.15704898
 12       -3.78843506     3.30232789    -3.79042120
 13       -1.79110569    -1.20073535     4.03963826
 14        2.06243294     0.89760392     5.60178021
 15        5.28956960     2.45060220     2.57907840
 16        4.63925516     1.85908132    -2.02317824
 17        0.75882867    -0.23257947    -3.58882437
 18       -4.43309615    -3.60956310    -3.81409144
 19       -7.06647030    -2.68891054    -0.48998461
 20       -5.57878413    -0.84353960     2.09656488
 END

*START
 STATUS 2
 SPECIES NONLINTS
 GEOM
  1        5.87535321     0.41787962     0.12023761
  2        3.59487191    -0.22529371    -0.99863029
  3        1.48215956    -0.75042876     0.51087034
  4        1.69233257    -0.64941464     3.14750266
  5        3.98187167    -0.01176215     4.25379884
  6        6.06970950     0.52700070     2.74397568
  7       -0.91682500    -1.41480506    -0.69562059
  8       -3.29706350    -1.21617827     0.43909739
  9       -4.80053833     1.39550224    -1.38789620
 10       -5.53716466     2.98167276     0.04523375
 11       -0.73721393    -2.06993552    -3.07861706
 12       -4.78315678     0.82743984    -3.60713587
 13        0.09279177    -1.10917994     4.33613088
 14        4.14240341     0.05438788     6.29233339
 15        7.85420144     1.02658583     3.61463228
 16        7.50087510     0.83876613    -1.04907127
 17        3.42244182    -0.30265656    -3.03490920
 18       -2.38794988    -1.85108310    -3.88745930
 19       -4.68263071    -2.62022704    -0.13290600
 20       -3.35877438    -0.68817523     2.40884540
 END

# end of start section

*PATH

 SCALEMASS  1.00

 RODS ON

 INTMU   3
 SSTEP   0.005
 INH     10

 SRANGE

  SLP   1.51
  SLM  -1.51
 END
```

```
 RPM       pagem

 SIGN    PRODUCT

 IDIRECT   1

 COORD  CURV3

 INTDEF
5-6 18-19 5-6-1 9-12-18
2-1 3-2 4-3 5-4 6-1 7-3 8-7 9-8 10-9 11-7 12-9 13-4
14-5 15-6 16-1 17-2 18-11 19-8 20-8 3-2-1 4-3-2 5-4-3
6-1-2 7-3-2 8-7-3 9-8-7 10-9-8 11-7-3 12-9-8 13-4-3
14-5-4 15-6-1 16-1-2 17-2-1 18-11-7 19-8-7 20-8-7
4-3-2-1 5-4-3-2 6-1-2-3 7-3-2-1 8-7-3-2 9-8-7-3
10-9-8-7 11-7-3-2 12-9-8-7 13-4-3-2 14-5-4-3 15-6-1-2
16-1-2-3 17-2-1-6 18-11-7-3 19-8-7-3 20-8-7-3
 END

 FREQSCALE 0.967

 PRPATH
  COORD 8 9
  INTERVAL 1
  XMOL
 END

*TUNNEL

QUAD
 NQE   40
 NQTH  40
END

 SCT

*RATE

  FORWARDK

  SIGMAF       1
  CVT
  PRDELG ON
# PRGIGT ON

  TEMP
    195.15
    273.15
    298.15
    350
  END
```

esp.fu70

```
*GRGENERAL

  GRRESTART
  RSTTOL 0.00001
```

```
*GRSTART

 CHARGE      0
 MULTIPLICITY  1

*GRREACT1

 CHARGE      0
 MULTIPLICITY  1

*GRPROD1

 CHARGE      0
 MULTIPLICITY  1

*GRCOMMON

 GRENER
    #p M062X/6-311+G** FCHK NOSYMM UNITS=AU
    scrf=(pcm,solvent=dichloromethane)
    scf=tight
    int(grid=ultrafine)
 END

 GRFIRST
    #p M062X/6-311+G** FORCE FCHK NOSYMM UNITS=AU
    scrf=(pcm,solvent=dichloromethane)
    scf=tight
    int(grid=ultrafine)
 END

 GRSEC
    #p M062X/6-311+G** FREQ=NORAMAN FCHK NOSYMM UNITS=AU
    scrf=(pcm,solvent=dichloromethane)
    scf=tight
    int(grid=ultrafine)
 END

 GRLINK0
   %chk=g09.chk
   %nproc=20
   %mem=40gb
 END
```

esp.fu71

```
%nproc=20
%mem=40gb
%chk=g09.chk
#p M062X/6-311+G** opt fchk NOSYMM
scf=tight int(grid=ultrafine)
scrf=(pcm,solvent=dichloromethane)

sm for decarboxylation

0 1
 C    2.270371    0.323739   -0.065274
 C    1.050840    0.009252   -0.651796
 C   -0.066128   -0.256670    0.153094
 C    0.057069   -0.219337    1.548891
```

C	1.279919	0.093829	2.130141
C	2.385292	0.368527	1.324638
C	-1.348950	-0.579383	-0.486435
C	-2.608222	-0.467702	0.125522
C	-3.330390	0.527940	-0.733064
O	-3.954824	1.409643	-0.227422
O	-1.289561	-0.890557	-1.753928
O	-3.333916	0.397547	-1.953231
H	-0.793704	-0.455365	2.179226
H	1.373000	0.118937	3.210700
H	3.338769	0.614204	1.781840
H	3.130999	0.538252	-0.690176
H	0.943608	-0.025592	-1.730320
H	-2.721475	-0.364532	-2.236546
H	-3.327577	-1.245456	-0.125864
H	-2.649464	-0.119852	1.149476

esp.fu73

%nproc=20
%mem=40gb
%chk=g09.chk
#p M062X/6-311+G** opt fchk NOSYMM
scf=tight int(grid=ultrafine)
scrf=(pcm,solvent=dichloromethane)

product from decarboxylation

0 1

C	2.270371	0.323739	-0.065274
C	1.050840	0.009252	-0.651796
C	-0.066128	-0.256670	0.153094
C	0.057069	-0.219337	1.548891
C	1.279919	0.093829	2.130141
C	2.385292	0.368527	1.324638
C	-1.348950	-0.579383	-0.486435
C	-2.608222	-0.467702	0.125522
C	-4.052557	1.523583	-1.591650
O	-4.611047	2.316217	-0.896804
O	-1.289561	-0.890557	-1.753928
O	-3.715536	0.902757	-2.595052
H	-0.793704	-0.455365	2.179226
H	1.373000	0.118937	3.210700
H	3.338769	0.614204	1.781840
H	3.130999	0.538252	-0.690176
H	0.943608	-0.025592	-1.730320
H	-2.175625	-0.588285	-2.155937
H	-3.327577	-1.245456	-0.125864
H	-2.649464	-0.119852	1.149476

esp.fu75

%nproc=20
%mem=40gb
%chk=g09.chk
#p M062X/6-311+G** opt=(ts,calcfc,noeigentest) fchk NOSYMM
int(grid=ultrafine)
scrf=(pcm,solvent=dichloromethane)

ts for decarboxylation

0 1

C	2.270371	0.323739	-0.065274
C	1.050840	0.009252	-0.651796
C	-0.066128	-0.256670	0.153094
C	0.057069	-0.219337	1.548891
C	1.279919	0.093829	2.130141
C	2.385292	0.368527	1.324638
C	-1.348950	-0.579383	-0.486435
C	-2.608222	-0.467702	0.125522
C	-3.512487	0.778996	-0.949560
O	-4.070977	1.571630	-0.254713
O	-1.289561	-0.890557	-1.753928
O	-3.368029	0.430835	-2.117352
H	-0.793704	-0.455365	2.179226
H	1.373000	0.118937	3.210700
H	3.338769	0.614204	1.781840
H	3.130999	0.538252	-0.690176
H	0.943608	-0.025592	-1.730320
H	-2.175625	-0.588285	-2.155937
H	-3.327577	-1.245456	-0.125864
H	-2.649464	-0.119852	1.149476

NMR Integration Macros

Macro “hsam1”

The listing below shows a sample macro for the output of ^{13}C NMR integrations. The spectra were first carefully phased by hand and the phases were recorded for use in the macro. The integration cut points shown in the macro were in each case used for both the sample and the standard.

```
$filename='/nmrdata/singleton/biswas/Hannah/20_percent_conversion_spectra.fid'
$filenameshort='Hannah-sam1'
rt($filename)

lvl=-0.04
rp=-8.6
lp=25.5
"my cuts based on biggest 50% linewidth for each peak"
"plus first is increased due to bad peak"
$cut[1]=10.1
$cut[2]=10.3
$cut[3]=9.7
$cut[4]=10.3
$cut[5]=11.
$cut[6]=11

setlimit('fn',2097152,8,2)
fn=1048576
wft('all')
wc=550
axis='p'

"For this program the argument is the number of spectra to be worked up in the array"
if ($#<1) then $numspec=6 else $numspec=$1 endif
$multiplier=1

$spectrum=1
repeat
```

```
ds($spectrum)
echo('new spectrum')

"spectrum-specific phases"
if (2>1) then
  if ($spectrum=1) then rp=-8.3 endif
  if ($spectrum=2) then rp=-8.7 endif
  if ($spectrum=3) then rp=-8.9 endif
  if ($spectrum=4) then rp=-9.2 endif
  if ($spectrum=5) then rp=-9.2 endif
  if ($spectrum=6) then rp=-9.2 endif
endif

"First, I want to get the full spectrum, set some basics and set the shifts"
$totalwidth=0
$sp=sp $wp=wp
vp=12 f intmod='partial' cz vs=160 th=5 nm

"count lines in case something is going wrong and exit if so"
nll('pos',20):$count
echo('here1')
if ($count<5 or $count>15) then
  text
  echo('Problem with wrong number of peaks.')
  return
endif

"----------------------------Setting shifts-------------------------"
"get carbonyl set to 190p then find chlororm and set it at 77.00"
getll(1):$ht,$freq
cr=$freq
rl(196.9p)
sp=76.0p wp=4p
repeat
  nll('pos',10):$count
  if ($count<3) then th=th-1 endif
  if ($count>3) then th=th+1 endif
  nll('pos',10):$count
until ($count=3)
getll(2):$ht,$freq
cr=$freq rl(77.00p) f
"----------------------------------------------------------------------"

"----------------------------Cutting integrations---------------"
"to turn off this section make the next line false, to turn it on make the line true"
if (2>1) then

cz
"1 now focus on carbonyl ono far left and cut it"
sp=194p wp=6p
repeat
  nll('pos',144):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',144):$count
until ($count=1)
$i=1
repeat
  getll($i):$ht,$freq
  dres($freq):$lw
  write('file','/home/singleton/dsingle/linewidths1','%.3f ',$lw)
  $totalwidth=$totalwidth+$lw
```

```
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>1)

"2 now focus on second peak from the left"
sp=135p wp=2p
repeat
  nll('pos',100):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',100):$count
until ($count=1)
$i=2
repeat
  getll($i-1):$ht,$freq
  dres($freq):$lw
  write('file','/home/singleton/dsingle/linewidths2','%.3f ',$lw)
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>2)

"Now focus on cutting the third peak, cut them"
sp=131p wp=3p
repeat
  nll('pos',20):$count
  if ($count<1) then th=th-1 endif
  if ($count>1) then th=th+1 endif
  nll('pos',20):$count
until ($count=1)
$i=3
repeat
  getll($i-2):$ht,$freq
  dres($freq):$lw
  write('file','/home/singleton/dsingle/linewidths3','%.3f ',$lw)
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
  $i=$i+1
until ($i>3)

"now focus on cutting peaks 4"
sp=125p wp=5p
repeat
  nll('pos',80):$count
  if ($count<2) then th=th-1 endif
  if ($count>2) then th=th+1 endif
  nll('pos',80):$count
until ($count=2)
$i=4
  getll(1):$ht,$freq
  dres($freq):$lw
  write('file','/home/singleton/dsingle/linewidths4','%.3f ',$lw)
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
$i=5
  getll(2):$ht,$freq
  dres($freq):$lw
  write('file','/home/singleton/dsingle/linewidths5','%.3f ',$lw)
  $totalwidth=$totalwidth+$lw
  z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)
```

```
"Focus on cutting peaks 6 "
sp=23p wp=6p
repeat
   nll('pos',70):$count
   if ($count<1) then th=th-1 endif
   if ($count>1) then th=th+1 endif
   nll('pos',70):$count
until ($count=1)
$i=6
   getll(1):$ht,$freq
   dres($freq):$lw
   write('file','/home/singleton/dsingle/linewidths6','%.3f ',$lw)
   $totalwidth=$totalwidth+$lw
   z($freq+$cut[$i]*$multiplier,$freq-$cut[$i]*$multiplier)



endif
"---------------------------------------------------------------"

echo('The average line width is ',$totalwidth/6)

"--------------------------Output integrals-----------------------"
"to turn off this section make the next line false, to turn it on make the line true"
if (2>1) then
   intmod='partial'
   f
   nll('pos',20):$count
   printon
   shell('date')
   text(file)
   echo('The average line width is ',$totalwidth/6)
   nli
   setint(4,2000)
   printoff('/home/singleton/dsingle/vnmrsys/maclib/temp1')
   shell('cat /home/singleton/dsingle/vnmrsys/maclib/temp1 >> /home/singleton/dsingle/vnmrsys/maclib/temphsam1')

endif
"---------------------------------------------------------------"

$spectrum=$spectrum+1
until ($spectrum>$numspec)

sp=$sp wp=$wp
sp=127p wp=1.1p intmod='full'
is=8000000
vs=1600
```

Macro “hrakinh1”

The listing below shows a sample macro for the output of ^{1}H NMR integrations for kinetics reactions. The spectra were first carefully phased by hand and the phases were recorded for use in the macro. The integration cut points were varied from spectrum to spectrum due to slight changes in the positions of peaks with concentration.

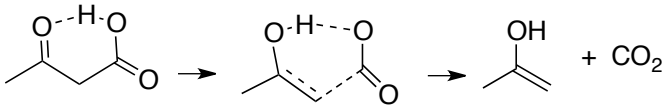
```
$filename='/nmrdata/singleton/haziz/03012015HRAKineticsH0hr.fid'
rt($filename)
fn=131072
wft
```

```
rp=113
lp=11
lvl=0
f
cr=7.26p
nl
nl
rl(7.26p)
intmod='partial'
cz
z(12.38p,12.26p)
z(8.01p,7.986p,7.986p,7.966p)
z(7.966p,7.94p)
z(7.83p,7.78p)
z(7.695p,7.63p)
z(7.595p,7.549p)
z(7.549p,7.462p)
z(7.462p,7.447p,7.447p,7.41p)
z(5.74p,5.712p)
z(4.11p,4.07p)
z(2.625p,2.609p)
is=3000
vs=300
sp=.5p
wp=13p
setint(.3,1)
setint(2,1000)
shell('rm /home/singleton/dsingle/vnmrsys/maclib/tempzh')
printon
shell('date')
text(file)
nli
setint(2,1000)
printoff('/home/singleton/dsingle/vnmrsys/maclib/temp1')
shell('cat /home/singleton/dsingle/vnmrsys/maclib/temp1 >> /home/singleton/dsingle/vnmrsys/maclib/tempzh')
$filename='/nmrdata/singleton/haziz/03012015HRAKineticsH1hr.fid'
rt($filename)
fn=131072
wft
rp=113
lp=11
lvl=0
f
cr=7.26p
nl
nl
rl(7.26p)
intmod='partial'
cz
z(12.38p,12.26p)
z(8.01p,7.986p,7.986p,7.966p)
z(7.966p,7.94p)
z(7.83p,7.78p)
z(7.695p,7.63p)
z(7.595p,7.549p)
z(7.549p,7.462p)
z(7.462p,7.447p,7.447p,7.41p)
z(5.74p,5.712p)
z(4.11p,4.07p)
z(2.625p,2.609p)
is=3000
vs=300
```

```
sp=.5p
wp=13p
setint(.3,1)
setint(2,1000)
printon
shell('date')
text(file)
nli
setint(2,1000)
printoff('/home/singleton/dsingle/vnmrsys/maclib/temp1')
shell('cat /home/singleton/dsingle/vnmrsys/maclib/temp1 >> /home/singleton/dsingle/vnmrsys/maclib/tempzh')
```

Computational Methods Evaluation Studies

The suitability of DFT methods for studying the decarboxylation of the experimental system **1** was explored by considering the model decarboxylation of formylacetic acid (**FA**). We first explored how well a series of method / basis set combinations reproduced the energies of the decarboxylation transition state (**TS-FA**) and the products (**Enol** + CO_2). The results are shown in the table below. The lowest average absolute errors were observed in wB97xd/6-311+G** and M06-2X/6-311+G** calculations. These methods were then explored in more detail for their accuracy in the area of the decarboxylation transition state.



FA **TS-FA** **Enol**

Table S2.

			Average				Average
	G4		absolute		M06/6-31+G**		absolute
FA	-342.259169		error	**FA**	-342.166632		error
TS-FA	-342.217760	**26.0**		**TS-FA**	-342.131819	21.8	3.4
Enol+CO2	-153.727172	**-2.1**		**Enol+CO2**	-153.668085	0.5	
	-188.535266				-188.497672		
	G3B3				M062X/6-31+G**		
FA	-342.202920	**Erel**	0.2	**FA**	-342.201294		
TS-FA	-342.162014	**25.7**		**TS-FA**	-342.162573	24.3	3.4
Enol+CO2	-153.701852	**-2.1**		**Enol+CO2**	-153.692419	3.0	
	-188.504351				-188.504123		
	PBE0/6-31+G**				M062X/6-311+G**		
FA	-341.972944		4.9	**FA**	-342.294966		
TS-FA	-341.936978	22.6		**TS-FA**	-342.257163	23.7	1.8
Enol+CO2	-153.588004	4.3		**Enol+CO2**	-153.733117	-0.6	
	-188.378120				-188.562867		
	B3PW91/6-31+G**				M062X/6-311++G**		
FA	-342.212879		3.8	**FA**	-342.295136		
TS-FA	-342.178831	21.4		**TS-FA**	-342.257281	23.8	1.8
Enol+CO2	-153.708877	1.0		**Enol+CO2**	-153.733232	-0.6	
	-188.502485				-188.562867		
	mPW1PW91/6-31+G**				M062X/6-31++G(2d,2p)		
FA	-342.256980		4.2	**FA**	-342.224707		
TS-FA	-342.220973	22.6		**TS-FA**	-342.186268	24.1	2.4
Enol+CO2	-153.725924	2.9		**Enol+CO2**	-153.702178	1.0	

	-188.526384				-188.520979		
	wB97xd/6-31+G**				M062X/aug-cc-pvdz		
FA	-342.235664		3.1	**FA**	-342.250857		
TS-FA	-342.195615	25.1		**TS-FA**	-342.212116	24.3	2.8
Enol+CO2	-153.715193	3.3		**Enol+CO2**	-153.710795	1.9	
	-188.515158				-188.537112		
	wB97xd/6-311+G**				M062X/cc-pvtz		
FA	-342.319353		1.5	**FA**	-342.326140		
TS-FA	-342.280450	24.4		**TS-FA**	-342.289191	23.2	2.0
Enol+CO2	-153.751156	-0.7		**Enol+CO2**	-153.747990	-0.9	
	-188.569298				-188.579607		
	B3LYP/6-31+G**/GD3				B3LYP/6-31+G**		
FA	-342.354194			**FA**	-342.348497		
TS-FA	-342.319851	21.6	4.0	**TS-FA**	-342.313876	21.7	2.7
Enol+CO2	-153.772851	1.5		**Enol+CO2**	-153.771008	-0.8	
	-188.579021				-188.578828		
	B3LYP/6-31G*						
FA	-342.319513						
TS-FA	-342.285307	21.5	3.7				
Enol+CO2	-153.748938	0.8					
	-188.569348						

The minimum-energy path for the decarboxylation of **FA** was explored in the area of **TS-FA** using Gaussrate / Polyrate, and a series of points were picked out at s = -0.4, -0.3, -0.2, -0.1, 0.0, 0.1, 0.2, 0.3, and 0.4 Å relative to **TS-FA**, using M06-2X / 6-311+G** for the Polyrate calculation. These structures were then used for CCSD(T)/jun-cc-pvtz, M06-2X/6-311+G**, and wB97xd/6-311+G** single-point calculations. The results are summarized in the table below. The average absolute error was slightly lower for the M06-2X calculations, and the M06-2X energies were particularly accurate in the area of the transition state. Based on this, the M06-2X/6-311+G** calculations were used for the study of the decarboxylation of **1**.

Table S3.

	CCSD(T)/jun-cc-pvtz		M062X/6-311+G**		absolute error	wB97xd/6-311+G**		absolute error
-0.4	-341.875998	**-5.74**	-342.3345685	-5.03	0.71	-342.3575785	-4.8	0.93
-0.3	-341.871297	**-2.79**	-342.3303309	-2.37	0.42	-342.3533954	-2.2	0.61
-0.2	-341.868501	**-1.03**	-342.3279271	-0.86	0.17	-342.351062	-0.7	0.32
-0.1	-341.867214	**-0.23**	-342.3268514	-0.19	0.04	-342.3501107	-0.1	0.11
0	-341.866855	**0.00**	-342.3265555	0.00	0.00	-342.3499222	0.0	0.00
0.1	-341.867109	**-0.16**	-342.3268021	-0.15	0.00	-342.3502021	-0.2	0.02
0.2	-341.867792	**-0.59**	-342.3274712	-0.57	0.01	-342.3507621	-0.5	0.06
0.3	-341.868811	**-1.23**	-342.3284967	-1.22	0.01	-342.3515717	-1.0	0.19
0.4	-341.870117	**-2.05**	-342.329811	-2.04	0.00	-342.352618	-1.7	0.35
FA	-341.910980	**-27.69**	-342.3674699	-25.67	2.01	-342.3917736	-26.3	1.43
Enol+CO2	-153.575995	**-26.64**	-153.7901879	-24.17	2.47	-153.8081864	-24.8	1.88
	-188.333309		-188.5748808			-188.5811893		
					ave. abs. error			
					0.53			0.54

Calculated Structures and Complete Energies

In addition to the structures given here, a number of other structures were obtained in exploratory studies. For example, the s-trans monomer of **1** and hydrogen-bonded dimers of **1** were obtained, but these were judged to be of little relevance based on either their energetics or prior experimental studies.

M062X/6-311+G**/PCM(CH_2Cl_2) Structures for Reaction of 1

Starting structure 4

Hannah SM
M062X/6-311+G**
E(RM062X) = -573.407197806

Zero-point correction= 0.154378 (Hartree/Particle)
Thermal correction to Energy= 0.164617
Thermal correction to Enthalpy= 0.165561
Thermal correction to Gibbs Free Energy= 0.116418
Sum of electronic and ZPE= -573.252820
Sum of electronic and thermal Energies= -573.242581
Sum of electronic and thermal Enthalpies= -573.241637
Sum of electronic and thermal Free Energies= -573.290779

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	103.299	37.972	103.429

6 -3.247537 0.927367 -0.065135
6 -1.885806 1.187451 -0.041519
6 -0.970051 0.131146 0.015650
6 -1.433105 -1.187393 0.051484
6 -2.798963 -1.444231 0.031273
6 -3.704551 -0.389331 -0.028263
6 0.479220 0.460660 0.038609
6 1.477295 -0.681202 0.028303
6 2.967133 -0.355083 -0.025426
8 3.776880 -1.242231 -0.092719
8 0.850113 1.622864 0.065928
8 3.336646 0.916795 0.011902
1 -0.742538 -2.020241 0.098576
1 -3.154864 -2.466427 0.061327
1 -4.768720 -0.592346 -0.046332
1 -3.954166 1.746660 -0.112523
1 -1.514010 2.204122 -0.068782
1 2.532181 1.483158 0.050889
1 1.323366 -1.290635 0.923984
1 1.267834 -1.340019 -0.817882

Enol 1'

M062X/6-311+G**
E(RM062X) = -573.407993516

Zero-point correction= 0.155304 (Hartree/Particle)
Thermal correction to Energy= 0.165258

Thermal correction to Enthalpy= 0.166202
Thermal correction to Gibbs Free Energy= 0.118886
Sum of electronic and ZPE= -573.252690
Sum of electronic and thermal Energies= -573.242736
Sum of electronic and thermal Enthalpies= -573.241792
Sum of electronic and thermal Free Energies= -573.289108

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	103.701	38.184	99.585

C,0,2.3489408403,0.1669828466,-0.0225159074
C,0,1.1161857454,0.0883787938,-0.659356436
C,0,-0.0523417252,-0.0771879205,0.0899030239
C,0,0.0320474507,-0.1843592395,1.4816128078
C,0,1.266507898,-0.1120745653,2.1132296915
C,0,2.4267853034,0.067992973,1.3635693602
C,0,-1.3547971014,-0.1363030194,-0.6060681365
C,0,-2.5430650921,0.1453958787,-0.0043738605
C,0,-3.7727470575,0.0656582234,-0.757028484
O,0,-4.8661189477,0.3598628609,-0.0437894256
O,0,-1.2606379781,-0.4709703799,-1.8901849791
O,0,-3.8525423633,-0.2354325479,-1.9443128148
H,0,-0.8609444881,-0.3483238708,2.0721317176
H,0,1.3242847452,-0.2042444356,3.1909000612
H,0,3.38867439,0.1248742377,1.8589284736
H,0,3.2490409425,0.3043037549,-0.6093081657
H,0,1.0506796754,0.1636552697,-1.7371458624
H,0,-2.1666810749,-0.460653529,-2.27295664
H,0,-2.587106804,0.4556912034,1.0269926868
H,0,-5.6351933585,0.287437466,-0.6270411107

TS 5‡

Hannah decarboxylation TS 6-311+G**
M062X/6-311+G**
E(RM062X) = -573.367652975

Zero-point correction= 0.152249 (Hartree/Particle)
Thermal correction to Energy= 0.162302
Thermal correction to Enthalpy= 0.163246
Thermal correction to Gibbs Free Energy= 0.115233
Sum of electronic and ZPE= -573.215404
Sum of electronic and thermal Energies= -573.205351
Sum of electronic and thermal Enthalpies= -573.204407
Sum of electronic and thermal Free Energies= -573.252420

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	101.846	37.908	101.051

6 -2.846412 0.928870 -0.722591
6 -1.531328 1.153101 -0.344455
6 -0.806882 0.142401 0.302753
6 -1.420528 -1.086309 0.577799
6 -2.737796 -1.302122 0.200018
6 -3.449502 -0.297776 -0.451944
6 0.582708 0.390394 0.690514
6 1.536462 -0.601060 0.946428
6 2.720512 -0.402091 -0.480516
8 2.857337 -1.455914 -1.030387
8 0.936514 1.653017 0.694527
8 3.125013 0.740693 -0.484924
1 -0.883116 -1.863691 1.105205
1 -3.211689 -2.250625 0.418882
1 -4.477743 -0.470365 -0.746603
1 -3.401680 1.707666 -1.230098
1 -1.052422 2.100141 -0.556319
1 1.911839 1.709870 0.622549
1 2.279520 -0.360559 1.702257
1 1.200971 -1.627241 0.942360

VTS 7‡

Hannah decarboxylation TS 6-311+G** CVTS
M062X/6-311+G**
E(RM062X) = -573.367719242

Zero-point correction= 0.152290 (Hartree/Particle)
Thermal correction to Energy= 0.162290
Thermal correction to Enthalpy= 0.163234
Thermal correction to Gibbs Free Energy= 0.115482
Sum of electronic and ZPE= -573.215429
Sum of electronic and thermal Energies= -573.205429
Sum of electronic and thermal Enthalpies= -573.204485
Sum of electronic and thermal Free Energies= -573.252238

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	101.839	37.760	100.504

6 3.108938 0.221183 0.063290
6 1.902832 -0.119930 -0.528908
6 0.784492 -0.398688 0.269998
6 0.894838 -0.343939 1.665613
6 2.106481 -0.006749 2.250979
6 3.211272 0.278534 1.451942
6 -0.483177 -0.747155 -0.370234
6 -1.750554 -0.632156 0.226626
6 -2.534265 0.726620 -0.725662
8 -2.930504 1.577406 0.021911
8 -0.391727 -1.093089 -1.628403
8 -2.529750 0.436774 -1.907453
1 0.047977 -0.586190 2.294453
1 2.191405 0.028542 3.329665
1 4.155390 0.543320 1.912843
1 3.969026 0.444922 -0.555166
1 1.811547 -0.160217 -1.606484
1 -1.266523 -0.965868 -2.055502
1 -2.470943 -1.392960 -0.064514
1 -1.778353 -0.357814 1.270801

enol 2

M062X/6-311+G**
E(RM062X) = -384.815697799

Zero-point correction= 0.139026 (Hartree/Particle)
Thermal correction to Energy= 0.146607
Thermal correction to Enthalpy= 0.147551
Thermal correction to Gibbs Free Energy= 0.106676

Sum of electronic and ZPE= -384.676672
Sum of electronic and thermal Energies= -384.669091
Sum of electronic and thermal Enthalpies= -384.668147
Sum of electronic and thermal Free Energies= -384.709022

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	91.997	29.894	86.030

C,0,3.0855833263,0.2873919517,0.0689680743
C,0,1.8749656565,-0.0846856423,-0.5070621294
C,0,0.7862155506,-0.433467361,0.2971489173
C,0,0.9400194453,-0.4260737582,1.6873300291
C,0,2.1496007166,-0.0542846291,2.2599428577
C,0,3.2265442915,0.3066108713,1.4528085095
C,0,-0.5073497927,-0.7997379808,-0.3270604562
C,0,-1.6986648111,-0.6969033996,0.2678459945
O,0,-0.3472348318,-1.2388954115,-1.6097080054
H,0,0.1176382377,-0.7304530796,2.3235900665
H,0,2.2559437581,-0.0572412753,3.3382121926
H,0,4.1705238834,0.5928583214,1.9010249185
H,0,3.9197060974,0.5616126568,-0.5660151116
H,0,1.7658713411,-0.099758419,-1.5838904881
H,0,-1.2107935791,-1.3895312076,-2.0088201856
H,0,-2.6073259129,-0.99076038,-0.2441829626
H,0,-1.7859443769,-0.3002812572,1.2682777789

CO_2

M062X/6-311+G**
E(RM062X) = -188.577399327

Zero-point correction= 0.011872 (Hartree/Particle)
Thermal correction to Energy= 0.014481
Thermal correction to Enthalpy= 0.015425
Thermal correction to Gibbs Free Energy= -0.008807
Sum of electronic and ZPE= -188.565527
Sum of electronic and thermal Energies= -188.562919
Sum of electronic and thermal Enthalpies= -188.561974
Sum of electronic and thermal Free Energies= -188.586207

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	9.087	6.803	51.001

C,0,0.,0.,0.
O,0,0.,0.,1.154767858
O,0,0.,0.,-1.154767858

9‡ and its starting material, M062X/6-311+G**/PCM(CH_2Cl_2)

Starting acid for 9‡

SM11
M062X/6-311+G**
E(RM062X) = -777.895967852

Zero-point correction= 0.157197 (Hartree/Particle)
Thermal correction to Energy= 0.169896
Thermal correction to Enthalpy= 0.170840
Thermal correction to Gibbs Free Energy= 0.115612
Sum of electronic and ZPE= -777.738771
Sum of electronic and thermal Energies= -777.726072
Sum of electronic and thermal Enthalpies= -777.725128
Sum of electronic and thermal Free Energies= -777.780356

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	106.611	46.462	116.237

C,0,2.4524623998,0.0184210985,0.0011452913
C,0,1.2357307209,0.0025911686,-0.6602551947
C,0,0.0396924504,-0.0035746133,0.0627630835
C,0,0.0620660477,0.0062520187,1.4588634234
C,0,1.2739568098,0.02215058,2.1359994986
C,0,2.4403773922,0.0278189897,1.3887553291
C,0,-1.2411546038,-0.0208945482,-0.7119535948
C,0,-2.5432606077,-0.0271056273,0.0584943932
C,0,-3.8593443543,-0.0448921417,-0.7142142103
O,0,-4.9037767817,-0.0512009503,-0.1195305113
O,0,-1.213251172,-0.0295136339,-1.9274973144
O,0,-3.8188136916,-0.0528120228,-2.0389621407
H,0,-0.8534822678,0.00175269,2.0360986398
H,0,1.3169800367,0.0299731508,3.2160485563
N,0,3.7345421076,0.0446969078,2.106107431
H,0,3.390223554,0.0234346433,-0.5365576899
H,0,1.2006962648,-0.0051478552,-1.7419379268
H,0,-2.8847904042,-0.0466541045,-2.3389792271
H,0,-2.5586365878,-0.8941879367,0.7249639286
H,0,-2.5745684952,0.8494125384,0.711957825
O,0,3.7071625679,0.0537660319,3.3177632938
O,0,4.7473046144,0.0484766162,1.4407641163

TS 9‡

M062X/6-311+G**
E(RM062X) = -777.855410188

Zero-point correction= 0.154632 (Hartree/Particle)
Thermal correction to Energy= 0.167140
Thermal correction to Enthalpy= 0.168085
Thermal correction to Gibbs Free Energy= 0.113203
Sum of electronic and ZPE= -777.700778
Sum of electronic and thermal Energies= -777.688270
Sum of electronic and thermal Enthalpies= -777.687326
Sum of electronic and thermal Free Energies= -777.742207

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	104.882	46.093	115.508

C,0,3.1196961731,0.2275280948,0.0560883297
C,0,1.9056920135,-0.098805034,-0.5256621072
C,0,0.7946619682,-0.3781864967,0.2787492462
C,0,0.9048200048,-0.3453232999,1.6726226531
C,0,2.1162013309,-0.0249322197,2.265531131
C,0,3.1937378008,0.2570521349,1.4406485442
C,0,-0.4846352031,-0.7170906853,-0.3638464545
C,0,-1.7451434233,-0.5872310847,0.2407754697
C,0,-2.5903709443,0.6720625452,-0.7733332319

O,0,-3.0679319666,1.5147413721,-0.0693833261
O,0,-0.3945340447,-1.0669678312,-1.6139676837
O,0,-2.53434731,0.3401682981,-1.9446081264
H,0,0.060039508,-0.5909443553,2.3019657444
H,0,2.2288505461,0.0013565393,3.34017397
N,0,4.489171888,0.6028840443,2.0688613815
H,0,3.9901122347,0.4566784544,-0.542539235
H,0,1.8101053146,-0.1272075326,-1.6027888343
H,0,-1.2724405062,-0.9085205848,-2.0430078308
H,0,-2.4564487798,-1.3729924023,-0.0056128715
H,0,-1.7673465149,-0.2656850179,1.2715913723
O,0,4.5420049476,0.6161352779,3.2792104893
O,0,5.4202889627,0.8531477831,1.33520237

8‡ and its starting material, gas phase

Starting acid for 8‡

M062X/6-311+G**
E(RM062X) = -573.394103691

Zero-point correction= 0.154472 (Hartree/Particle)
Thermal correction to Energy= 0.163884
Thermal correction to Enthalpy= 0.164828
Thermal correction to Gibbs Free Energy= 0.118529
Sum of electronic and ZPE= -573.239632
Sum of electronic and thermal Energies= -573.230220
Sum of electronic and thermal Enthalpies= -573.229276
Sum of electronic and thermal Free Energies= -573.275575

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	102.839	36.098	97.445

C,0,2.4541461114,0.0278290599,0.0184047513
C,0,1.2432632549,0.0011576485,-0.6564919889
C,0,0.0418181329,-0.0182313736,0.0578737655
C,0,0.0674643436,-0.0121104252,1.4545030542
C,0,1.2827587647,0.0124054991,2.1282772803
C,0,2.474270718,0.0332387556,1.4114731
C,0,-1.2324968803,-0.0495309598,-0.7161517089
C,0,-2.5398111436,-0.0414981215,0.0517387107
C,0,-3.8681779223,0.0080747624,-0.7129513045
O,0,-4.8929470922,0.0836038937,-0.1003388319
O,0,-1.2101273022,-0.0853742028,-1.9322245224
O,0,-3.8334426705,-0.0452738554,-2.0387164711
H,0,-0.8515822213,-0.0294691691,2.0272973614
H,0,1.2990341173,0.0157345057,3.2111375693
H,0,3.4209122492,0.0535754059,1.9384559825
H,0,3.3830886013,0.0444755312,-0.5383027777
H,0,1.2046294442,-0.0048392804,-1.7388973341
H,0,-2.9044052349,-0.0847267773,-2.3409156462
H,0,-2.5811281414,-0.9358259231,0.6816474335
H,0,-2.5515971289,0.8042050263,0.743661577

TS 8‡

M062X/6-311+G**
E(RM062X) = -573.355594192

Zero-point correction= 0.151700 (Hartree/Particle)
Thermal correction to Energy= 0.161417
Thermal correction to Enthalpy= 0.162361
Thermal correction to Gibbs Free Energy= 0.115275
Sum of electronic and ZPE= -573.203895
Sum of electronic and thermal Energies= -573.194177
Sum of electronic and thermal Enthalpies= -573.193233
Sum of electronic and thermal Free Energies= -573.240319

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	101.291	36.944	99.100

C,0,3.1446665493,0.1904269804,0.0713216637
C,0,1.9264687545,-0.1140825103,-0.5160145788
C,0,0.8089685984,-0.3748013896,0.2858152865
C,0,0.9308180422,-0.3428098324,1.6793362868
C,0,2.1532546279,-0.0416682856,2.2615017246
C,0,3.2583067383,0.2284133509,1.4590056182
C,0,-0.4730645918,-0.6905750105,-0.3549821044
C,0,-1.7343626496,-0.5661600261,0.2579081263
C,0,-2.6530847175,0.621820309,-0.8152990746
O,0,-3.2392205196,1.4073673543,-0.144606547
O,0,-0.4211848316,-1.0054175842,-1.613666748
O,0,-2.4986177317,0.2752923677,-1.9804815736
H,0,0.0794422682,-0.5746291402,2.3069436651
H,0,2.2463935587,-0.0218184143,3.3402598935
H,0,4.2114089107,0.4655703055,1.9167990056
H,0,4.0059113482,0.4016998919,-0.5504009718
H,0,1.8205702494,-0.144730875,-1.5929407939
H,0,-1.3163333309,-0.6987827225,-2.0085140399
H,0,-2.4337772646,-1.3689082756,0.0348948486
H,0,-1.7690240085,-0.2073564935,1.2762903133

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