Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Structure coordinates and negative frequencies of the transition states.

Structure 1

Atom	X	Y	Z
C	0.2901340	0.1828820	−0.7711520
C	−0.8518490	1.0511960	−0.3420670
C	−1.9168930	0.2741730	0.0511000
C	−1.4870400	−1.0513490	−0.1385870
O	−0.2621130	−1.1728900	−0.6078970
H	0.5132080	0.2996200	−1.8369900
O	−2.2093670	−2.1047400	0.1111260
O	−3.0892230	0.7587650	0.5002460
H	−3.7163410	0.0657990	0.7571410
O	−0.7271600	2.3544100	−0.3659640
H	−1.5210140	2.8115700	−0.0325390
C	1.5711770	0.3488290	0.0832550
C	2.7487370	−0.4968740	−0.4262210
H	1.8505800	1.4051840	−0.0134190
H	2.5724920	−1.5617550	−0.2002350
H	2.8314620	−0.3995780	−1.5135880
O	3.9720280	−0.0383640	0.0974430
H	4.0229280	−0.2036120	1.0490120
O	1.2792210	0.1369030	1.4508230
H	1.3726730	−0.8011450	1.6724590
H	−1.7586740	−2.9419050	−0.1060200

Structure TS1 (negative frequency= −741.03cm−1)

Atom	X	Y	Z
C	−0.6758290	0.9564630	−0.3673510
C	−1.8531330	0.3848050	−0.0157750
C	−1.8185900	−1.0675430	0.0054480
O	−0.7646190	−1.6634860	−0.2629110
O	−2.9612050	−1.6608450	0.3240190
O	−2.9276200	1.1534360	0.2760170
H	−3.6469240	0.6346770	0.6678790
O	−0.4212280	2.2702170	−0.4207940
H	−1.1913700	2.7815230	−0.1144150
C	1.6849900	0.0965860	−0.0319070
C	2.8459010	−0.8223640	−0.3954940
H	1.6298420	1.0106390	−0.8914640
H	2.6195990	−1.8114690	0.0249320
H	2.9502310	−0.9092270	−1.4834020
O	3.9762790	−0.2269970	0.2132530
H	4.7077390	−0.8554970	0.2829840
O	1.6970530	0.6035930	1.2094250
H	2.6252300	0.6268340	1.5166430
H	−2.8594590	−2.6299950	0.3278930
C	0.4638650	0.0747240	−0.7471700
H	0.4926100	−0.3908590	−1.7296250

Structure 2

Atom	X	Y	Z

C	-0.4820470	0.8434420	-0.3870560
C	-1.7222250	0.4416480	-0.0194950
C	-2.1584010	-0.9663110	-0.0220440
O	-1.4697640	-1.9312710	-0.3244440
O	-3.4451200	-1.0675160	0.3595260
O	-2.5862500	1.4302360	0.3610700
H	-3.4596900	1.0655720	0.5701350
O	-0.1150560	2.1442850	-0.3720650
H	-0.8618720	2.6951820	-0.0772330
C	1.8221720	-0.0748230	-0.0448840
C	3.1839420	-0.3913720	-0.5878470
H	3.1244940	-1.3151200	-1.1841080
H	3.4651200	0.4286640	-1.2674680
O	4.0293740	-0.5110930	0.5314150
H	4.9620410	-0.3719570	0.3153380
O	1.7380660	0.1403290	1.2055190
H	2.6410940	0.0363550	1.6126330
H	-3.7142000	-2.0029380	0.3450320
C	0.6108290	-0.0584580	-0.8761960
H	0.8871240	0.1617430	-1.9158470
H	0.2202720	-1.1020100	-0.8615130

Structure TS2 (negative frequency= -2055.67 cm-1)

Atom	X	Y	Z
C	0.5223090	-1.4156740	0.4036280
C	1.4598250	-0.4416090	-0.1671170
C	1.5576600	1.0542350	0.0729590
O	0.5417790	1.7113180	0.1739530
O	2.8047470	1.4863320	0.1358190
O	2.2304520	-1.0558940	-0.9619680
H	1.6507920	-2.0391320	-0.4774410
O	0.1743410	-1.1829170	1.7405760
H	0.6234250	-1.8192450	2.3153050
C	-1.5275270	-0.4750060	-0.5151500
C	-2.2711580	0.1266990	0.6412540
H	-3.1148240	-0.5362470	0.8867120
H	-1.6112740	0.1475410	1.5179450
O	-2.7558700	1.3896760	0.2294810
H	-2.3495230	2.1010650	0.7455170
O	-1.5233980	0.2084860	-1.5970300
H	-2.0068120	1.0630370	-1.4045020
H	2.8236050	2.4517300	0.2811140
C	-0.7443830	-1.7246110	-0.4682270
H	-1.2830470	-2.5247610	0.0449290
H	-0.4891090	-2.0441960	-1.4803210

Structure 3

Atom	X	Y	Z
C	0.8186250	-1.4655810	0.1129480
C	1.8441370	-0.3549730	-0.1844790
C	1.3648180	1.0886120	0.0650130

O	0.1727930	1.3696620	0.0274860
O	2.3451580	1.9414840	0.2661970
O	2.9535670	-0.5875130	-0.5930190
H	1.3381230	-2.4078590	-0.0876050
O	0.3885470	-1.3727770	1.4648700
H	1.0095120	-1.8277520	2.0520510
C	-1.4305180	-0.3586450	-0.5342170
C	-2.1647040	-0.1431530	0.7659630
H	-2.6464370	-1.0961020	1.0310910
H	-1.4572080	0.1020510	1.5593000
O	-3.1487260	0.8430070	0.5178850
H	-3.0613910	1.5940260	1.1213350
O	-1.9004310	0.2604710	-1.5420540
H	-2.6211140	0.8695000	-1.2072700
H	1.9947600	2.8458100	0.3733670
C	-0.4246890	-1.4269580	-0.8017640
H	-0.9619310	-2.3771730	-0.6608140
H	-0.1275800	-1.3729750	-1.8531440

Structure TS3 (negative ferquency =-1585.94 cm-1)

Atom	X	Y	Z
C	1.3199130	0.0248060	0.2319930
C	0.9500100	0.8931940	-0.9610810
C	-0.5417760	1.1726610	-0.7477350
C	-0.9427640	-0.0818280	-0.0021890
O	0.0504080	-0.5501900	0.6870620
H	1.5368570	1.8110000	-1.0307180
H	-1.1055700	1.3444900	-1.6660080
C	-2.2370760	-0.8044710	0.0650720
O	-2.3676530	-1.9053200	0.5434300
O	-3.2038060	-0.0388290	-0.4796270
H	-4.0539680	-0.5130450	-0.4296370
H	1.1226920	0.3047620	-1.8671420
O	-0.6287870	2.2720210	0.1619830
H	-1.5379890	2.6041150	0.2163530
C	2.4341370	-0.9358040	0.1386170
H	2.4006640	-1.7717720	0.8401240
O	2.8630290	-1.1985580	-1.1311440
H	3.3443090	-2.0374160	-1.1739570
H	2.8109060	0.3066220	1.1825870
O	1.7853160	0.7492170	1.4741960
H	1.5993790	1.7131730	1.5331350

Structure 4

Atom	X	Y	Z
C	1.6151320	-0.2028640	-0.1549960
C	1.2588060	1.2462020	-0.3024710
C	-0.2424320	1.1962840	-0.6799490
C	-0.6032750	-0.2293380	-0.2787770
O	0.4275970	-0.9591020	-0.1187210
H	1.3694400	1.7794490	0.6492980
H	-0.3757980	1.2340430	-1.7743570

C	-1.9357570	-0.9316380	-0.2877670
O	-2.0875140	-2.0699590	0.0678630
O	-2.8712610	-0.0954990	-0.7647920
H	-3.7303860	-0.5561170	-0.7941070
H	1.8637410	1.7546980	-1.0550000
O	-0.9731470	2.2096060	-0.0457920
H	-1.7526150	2.4475800	-0.5678930
C	2.7585520	-0.9019830	-0.0366340
H	2.7426860	-1.9846700	0.0612870
O	3.9274940	-0.2539980	-0.0443720
H	4.6783990	-0.8592780	0.0401100
H	-1.1919630	-0.1085790	2.7772540
O	-0.8576970	0.4104740	2.0318030
H	-1.2334380	1.3007310	2.0990520

Structure TS4 (negative ferquency=-1917.71cm-1)

Atom	X	Y	Z
C	1.4099720	-0.2167410	-0.0736830
C	1.1262810	1.1220360	-0.5132550
C	-0.3612790	1.2343910	-0.4804950
C	-0.7899290	-0.1168210	-0.1138640
O	0.2368850	-0.8817020	0.1910540
H	0.8392910	1.9898490	0.6209720
H	-0.9533780	1.7976290	-1.1962230
C	-2.1385450	-0.7284740	-0.0287300
O	-2.3330220	-1.8634450	0.3323960
O	-3.0680680	0.1658930	-0.4117310
H	-3.9473370	-0.2518440	-0.3664480
H	1.7615960	1.6403400	-1.2237980
O	-0.3716130	2.1194290	0.8901960
H	-0.8607920	2.9710730	0.9138250
C	2.5432980	-0.9638170	0.1310530
H	2.4670430	-1.9918080	0.4788000
O	3.7232140	-0.4269070	-0.1028110
H	4.4556250	-1.0448240	0.0538750

Structure 5

Atom	X	Y	Z
C	-1.5008910	-0.1785270	-0.1456130
C	-1.2381310	-1.1968310	0.7943320
C	0.1403780	-1.3743680	0.8031180
C	0.6530040	-0.4563230	-0.1193940
O	-0.3098240	0.2469290	-0.6986970
H	1.3880630	2.6337140	1.0262230
H	0.7250620	-2.0637170	1.3942420
C	2.0514110	-0.1509750	-0.5583540
O	2.3170160	0.7086300	-1.3600490
O	2.9102460	-0.9724660	0.0586200
H	3.8159320	-0.7679720	-0.2366670
H	-1.9819910	-1.7206530	1.3799180
O	1.0384290	1.8572550	1.4851320
H	1.2170980	2.0122940	2.4223870

C	-2.6411010	0.4447000	-0.6013000
H	-2.5666360	1.2256810	-1.3572620
O	-3.8109660	0.1031420	-0.1282560
H	-4.5447550	0.6066810	-0.5195690

Structure TS5 (negative ferquency=-1731.19 cm-1)

Atom	X	Y	Z
C	1.3986890	0.0486670	0.0722110
O	0.2029400	-0.6504660	0.1208090
C	-0.7787380	0.2529560	0.0387710
C	-0.2874050	1.5535650	0.0125090
C	1.1003840	1.4444680	0.0944770
C	-2.2085410	-0.1949470	-0.0379210
O	-2.3190150	-1.5214820	-0.0498430
O	-3.0942620	0.6238340	-0.0737110
C	2.6669100	-0.6163730	0.4628660
O	3.4276770	-0.5485970	-0.5186500
H	2.9526320	-1.0709810	1.4155090
H	-3.2618160	-1.7677310	-0.0962230
H	2.2784670	-0.0135530	-1.0543460
H	1.8303630	2.2450770	0.1077510
H	-0.8861590	2.4508560	-0.0590060

Structure 6

Atom	X	Y	Z
C	1.5652330	0.2173090	-0.7631910
O	0.2816620	-0.4258680	-0.7957070
C	-0.5624120	0.3246500	-0.1483320
C	-0.0034710	1.5605800	0.2640330
C	1.2992550	1.5344370	-0.1528350
C	-1.9831970	-0.1363690	0.0823520
O	-2.2072900	-1.3355570	-0.4351880
O	-2.7432780	0.5859240	0.6789710
C	2.5140560	-0.6552310	0.2062280
O	2.0522420	-1.2923320	1.0981470
H	3.5862060	-0.5735440	-0.0384580
H	-3.1306160	-1.6037900	-0.2667550
H	2.0492860	2.3057360	-0.0153240
H	-0.5379000	2.3375080	0.7935790
H	1.9895460	0.2045090	-1.7723470

Structure TS6 (negative frequency=-75.69 cm-1)

Atom	X	Y	Z
C	-2.4200090	0.3244670	0.1965100
O	-0.0176940	-0.3788990	1.4604230
C	0.5012760	0.2392710	0.5590270
C	-0.2095990	1.3768400	-0.1049750
C	-1.5892590	1.4101160	-0.0627550
C	1.9036810	-0.1697960	0.0143720
O	2.4466510	0.8574620	-0.6525830
O	2.3570290	-1.2599780	0.1984930

C	−2.1135010	−1.0779940	−0.2792950
O	−1.2801380	−1.2715420	−1.1366370
H	−2.7099440	−1.8845920	0.1753660
H	3.3356190	0.6148560	−0.9760180
H	−2.0680820	2.3845510	−0.1904410
H	0.3676680	2.1940030	−0.5305180
H	−3.4075700	0.4974180	0.6267000

Structure 7

Atom	X	Y	Z
C	2.6133770	1.0063620	−0.1676390
O	−0.9290000	−1.8088180	−0.1317360
C	−0.7466640	−0.6373320	−0.0126060
C	0.6703150	−0.0956850	0.4300070
C	1.2931850	1.2150980	0.1380740
C	−1.8578680	0.4402560	−0.0611620
O	−3.0549520	−0.1155820	−0.0615740
O	−1.5836480	1.6202430	−0.0639800
C	2.7872250	−0.3949550	−0.1872970
O	1.7038350	−1.0560040	0.0935020
H	3.6720710	−0.9895090	−0.3976820
H	−3.7442050	0.5750910	−0.0841630
H	0.7703450	2.1561900	0.2561040
H	0.5798400	−0.1524310	1.5325390
H	3.3800100	1.7416710	−0.3733770

Structure TS7 (negative frequencu= −731.43 cm−1)

Atom	X	Y	Z
C	2.6360610	0.9797630	0.0005690
O	−0.9992870	−1.8535410	−0.0500560
C	−0.7018000	−0.6453380	0.1367610
C	0.6674640	−0.1175390	0.0109800
C	1.2613600	1.1761430	0.0683850
C	−1.8962270	0.4605430	−0.0124510
O	−3.0460390	−0.1644630	−0.0432050
O	−1.6424820	1.6308810	−0.0841870
C	2.8245930	−0.4031220	−0.0750590
O	1.6574760	−1.0599650	−0.0538780
H	3.7135310	−1.0164660	−0.1567250
H	−3.7770680	0.4751830	−0.1505540
H	0.7155720	2.1083920	0.1033260
H	−0.5737910	−0.4219320	1.2883400
H	3.4157090	1.7288400	−0.0088980

Structure 8

Atom	X	Y	Z
C	2.6538820	1.0045940	0.0024220
O	−1.0042350	−1.8773940	−0.0280380
C	−0.3759590	−0.9278420	0.0843310
C	0.7563460	−0.1526070	0.0634890
C	1.2615300	1.1524720	0.1027750

C	−2.0837780	0.6962840	0.2717000
O	−3.0989380	−0.0866110	−0.0688470
O	−1.7008910	1.7421420	−0.1901240
C	2.9131130	−0.3532070	−0.0924020
O	1.7923760	−1.0646520	−0.0651870
H	3.8282420	−0.9229700	−0.1855640
H	−3.6929760	0.3479330	−0.7126110
H	0.6806810	2.0617560	0.1755810
H	−1.5839040	0.2429430	1.1577310
H	3.3917820	1.7942810	−0.0077730