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

Topography of the Free Energy Landscape on the Claisen-Schmidt Condensation: Solvent and Temperature Effect in the Rate-Controlling Step

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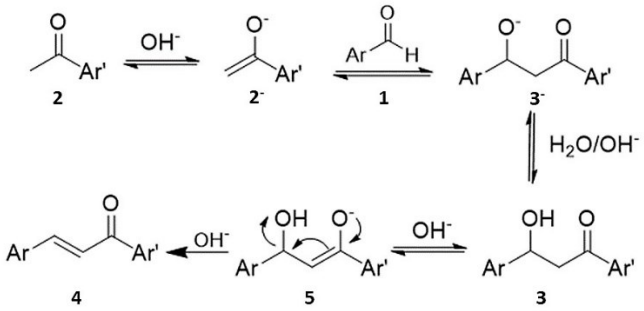
1. Theoretical and computational details

1.1. Claisen -Schmidt Condensation mechanism



Scheme S1. Steps of base-catalyzed chalcone 4 formation from benzaldehyde 1 and an acetophenone 2: (R1) First enolization, (R2) new C–C bond formation, (R3) proton equilibration, (R4) second enolization, and (R5) elimination (E_1cb) and C=C bond formation. Nomenclature and indexation used in Ref. [19] were kept to allow for easier comparison

1.2 Kramers Formulation

To account for dynamical effects of the solvent in a reactive process and to generalize to unimolecular and pseudo-unimolecular processes, the Kramers model considers a stochastic motion of the system where the solvent effect is added considering Brownian movements along the reaction path [1].

Assuming that the friction constant, μ (see below), is independent of time, the overall reaction rate constant k_{Obs} can be calculated as $k_{Obs} = \kappa_{Kr} k_{TST}$, where κ_{Kr} is the transmission factor obtained by Kramers2 as:

$$= \frac{1}{\omega^{\ddagger}} \left(\sqrt{\frac{\mu^2}{4} + \omega^{\ddagger 2}} - \frac{\mu}{2} \right). \quad \text{(S1)}$$

For the transition-state theory rate constant k_{TST} and variants see Ref.3 In (1), $\omega^{\ddagger}$ is the imaginary frequency of the transition state and the friction constant is given by $\mu = (6\pi r_{AB}/M)\eta$, where r_{AB} and M are the radius of the cage and the molecular mass of the transition-state, respectively.

Therefore, the equation of rate constant including quantum tunneling correction by Skodje-Truhlar and the Kramers transmission can be written as:

$$k_{obs} = \kappa_{ST} \kappa_{Kr} k_{TST} \quad \text{(S2)}$$

From k_{obs} is possible to obtain the intrinsic free energy barrier considering all physicochemical factors rewritten Equation S2 in terms of activation free energy, $\Delta G^{\ddagger}$, as:

$$\Delta G^{\ddagger} = -RT\ln\left(\frac{k_{obs}}{k_B T/h}\right) \quad \text{(S3)}$$

Where R is the ideal gas constant, T is the absolute temperature, k_B is Boltzmann's constant and h is Planck's constant.

Table S1. Rate constants for each step of chalcone formation, comparing our data in water and deuterated water environment at B3LYP/6-31+G(3df,3dp) level of theory and experimental data.

	Perrin 16	Guthrie 83	This work			
			Without Tunneling		With Tunneling	
			H_2O	D_2O	H_2O	D_2O
$k_{R1}(M^{-1}\cdot s^{-1})$	0.243	0.244	80.762	13.396	382.766	27.355
$k_{-R1}(s^{-1})$	4216	4240	36277	220.178	138433	449.267
$k_{R2}(M^{-1}\cdot s^{-1})$	1208	14454	8187	10052	8722	10702
$k_{-R2}(s^{-1})$	0.117	0.331	1333	982.192	1420	1046
$k_{R3}(s^{-1})$	2.684E+11	9.7724E+07	3.063E+10	3.452E+10	3.063E+10	3.452E+10
$k_{-R3}(M^{-1}\cdot s^{-1})$	1.617E+11	7.4131E+08	5.772E+12	6.257E+12	5.773E+12	6.257E+12
$k_{R4}(M^{-1}\cdot s^{-1})$	1.293	6.026	32.901	17.414	351.513	45.955
$k_{-R4}(s^{-1})$	2672	93.325	346.588	5.977	2249	15.706
$k_{R5}(s^{-1})$	22.833	0.398	1824	2794	1877	2893

Table S2: Rate constants for chalcone formation from acetophenone and benzaldehyde k_{Obs}, reversion from ketol to acetophenone and benzaldehyde $k_{\rightarrow 1+2}$ and chalcone formation from ketol $k_{\rightarrow 4}$.

Work	Solvent	$\frac{[OH^-]}{M}$	$\frac{k_{Obs}(298\ K)}{M^{-2}\cdot s^{-1}}$	$\frac{k_{3\rightarrow 1+2}(298\ K)}{M^{-1}\cdot s^{-1}}$	$\frac{k_{3\rightarrow 4}(298\ K)}{M^{-1}\cdot s^{-1}}$	$\frac{k_{3\rightarrow 1+2}}{k_{3\rightarrow 4}}$
Coombs 1940[6]	90% C_2H_5OH/H_2O	0.02	0.0458	-	-	-
Hammet 1943[7]	70% $C_4H_8O_2$ /H_2O	0.0507	0.0329	-	-	-
Noyce 1955[8]	90% C_2H_5OH /H_2O	0.02	0.0375	0.095	0.0258	4.45
Guthrie 1983[9]	CH_3CN/H_2O	0.10	0.0996	0.1940	0.0261	7.43

Gasull 2000[10]	65% C_2H_5OH /H_2O	0.0309	0.0246	-	-	-
Perrin-2016[5]	26% and 80% CH_3CN /H_2O	0.2	0.0111	0.0730	0.0110	6.64
This work R5 RLS	H_2O	-	0.0002	982.5023	360.5660	2.72

The temperature dependence for all elementary steps of base-catalyzed chalcone in aqueous environment using Aquilanti-Mundim formula are expressed as:

$$k_{R1} = 1.04 \times 10^{16} M^{-1} \cdot s^{-1} \left(1 + \frac{1762.8}{T}\right)^{-15.99} \quad \text{S4}$$

$$k_{-R1} = 5.82 \times 10^{7} s^{-1} \left(1 + \frac{369.5}{T}\right)^{-7.50} \quad \text{S5}$$

$$k_{R2} = 1.32 \times 10^{7} M^{-1} \cdot s^{-1} \left(1 - \frac{47.4}{T}\right)^{41.46} \quad \text{S6}$$

$$k_{-R2} = 3.80 \times 10^{12} s^{-1} \left(1 - \frac{69.3}{T}\right)^{82.17} \quad \text{S7}$$

$$k_{R3} = 2.61 \times 10^{9} s^{-1} \left(1 - \frac{195.6}{T}\right)^{4.16} \quad \text{S8}$$

$$k_{-R3} = 4.91 \times 10^{11} M^{-1} \cdot s^{-1} \left(1 - \frac{195.6}{T}\right)^{4.16} \quad \text{S9}$$

$$k_{R4} = 9.09 \times 10^{9} M^{-1} \cdot s^{-1} \left(1 + \frac{756.6}{T}\right)^{-13.48} \quad \text{S10}$$

$$k_{-R4} = 4.54 \times 10^{6} s^{-1} \left(1 + \frac{3455.7}{T}\right)^{-3.00} \quad \text{S11}$$

$$k_{R5} = 5.21 \times 10^{11} s^{-1} \left(1 - \frac{100.0}{T}\right)^{47.69} \quad \text{S12}$$

$$k_{-R5} = 8.91 \times 10^{7} M^{-1} \cdot s^{-1} \left(1 - \frac{96.1}{T}\right)^{48.26} \quad \text{S13}$$

The temperature dependence for all elementary steps of base-catalyzed chalcone in deuterated water environment using Aquilanti-Mundim formula are expressed as:

$$k_{R1} = 3.26 \times 10^{10} M^{-1} \cdot s^{-1} \left(1 + \frac{89.7}{T}\right)^{-79.49} \quad \text{S14}$$

$$k_{-R1} = 7.51 \times 10^{6} s^{-1} \left(1 - \frac{6.0}{T}\right)^{476.19} \quad \text{S15}$$

$$k_{R2} = 9.35 \times 10^{6} M^{-1} \cdot s^{-1} \left(1 - \frac{77.7}{T}\right)^{21.85} \quad \text{S16}$$

$$k_{-R2} = 4.07 \times 10^{12} s^{-1} \left(1 - \frac{70.0}{T}\right)^{82.30} \quad \text{S17}$$

$$k_{R3} = 2.61 \times 10^{9} s^{-1} \left(1 - \frac{195.6}{T}\right)^{4.16} \quad \text{S18}$$

$$k_{-R3} = 4.91 \times 10^{11} M^{-1} \cdot s^{-1} \left(1 - \frac{195.6}{T}\right)^{4.16} \quad \text{S19}$$

$$k_{R4} = 1.71 \times 10^{9} M^{-1} \cdot s^{-1} \left(1 + \frac{74.0}{T}\right)^{-78.55} \quad \text{S20}$$

$$k_{-R4} = 3.65 \times 10^{5} s^{-1} \left(1 + \frac{118.6}{T}\right)^{-29.98} \quad \text{S21}$$

$$k_{R5} = 2.47 \times 10^{12} s^{-1} \left(1 - \frac{75.5}{T}\right)^{70.57} \quad \text{S22}$$

$$k_{-R5} = 3.80 \times 10^{8} M^{-1} \cdot s^{-1} \left(1 - \frac{103.9}{T}\right)^{37.69} \quad \text{S23}$$

Calculated atomic coordinates (in angstroms), for all optimized structures of base-catalyzed chalcone reaction at B3LYP/6-31+G(3df,3dp) level of theory.

Acetophenone (2)

C	0.207182	-0.061270	-0.000074
C	-0.582392	-1.225509	-0.000017
C	-1.972809	-1.137845	0.000029
C	-2.595315	0.116877	0.000023
C	-1.820640	1.280681	-0.000029

C	-0.426756	1.193729	-0.000074
C	1.698315	-0.198723	-0.000132
C	2.556732	1.048372	0.000073
O	2.223277	-1.312163	0.000109
H	2.350871	1.663906	0.882375
H	-0.088579	-2.191239	-0.000014
H	-2.572879	-2.042906	0.000070
H	-2.299999	2.254892	-0.000033
H	0.158451	2.106813	-0.000112
H	2.351148	1.663986	-0.882236
H	3.607905	0.758071	0.000226
H	-3.679033	0.185915	0.000059

b3lyp:
Energy+ZPE (kcal/mol): -241461.496088102

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -241236.15258613002

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -241232.045539725

Frequencies: [58.1031, 149.2858, 153.4677, 218.5373, 366.7531, 412.2239, 430.8129, 467.2921, 594.9084, 604.9404, 628.2487, 697.2009, 742.8359, 773.412, 861.2237, 951.3553, 964.2825, 999.1936, 1012.8726, 1017.3087, 1043.4392, 1044.7524, 1093.4136, 1107.7093, 1181.1598, 1197.8432, 1279.9829, 1340.3946, 1361.393, 1391.7981, 1465.6731, 1471.6867, 1480.0341, 1525.0007, 1622.0389, 1641.5985, 1713.366, 3051.4188, 3115.3084, 3162.1351, 3189.532, 3197.8901, 3208.4818, 3218.5189, 3220.8839]

Deuterated Acetophenone (2)

C	0.207180	-0.061271	-0.000070
C	-0.582389	-1.225512	-0.000020
C	-1.972809	-1.137843	0.000030
C	-2.595320	0.116877	0.000020
C	-1.820641	1.280678	-0.000030
C	-0.426761	1.193728	-0.000070
C	1.698320	-0.198720	-0.000130
C	2.556729	1.048370	0.000070
O	2.223281	-1.312160	0.000110
H(Iso=2)	2.350869	1.663910	0.882380
H	-0.088578	-2.191241	-0.000010
H	-2.572879	-2.042913	0.000070
H	-2.300001	2.254887	-0.000030
H	0.158449	2.106809	-0.000110
H(Iso=2)	2.351149	1.663990	-0.882240
H(Iso=2)	3.607910	0.758071	0.000230
H	-3.679030	0.185916	0.000060

b3lyp:
Energy+ZPE (kcal/mol): -241467.49256410598

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -241242.059328347

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -241237.95667450503

Frequencies: [55.1059, 106.685, 151.2826, 207.2133, 347.1247, 410.2781, 419.2262, 447.7571, 540.2674, 553.4301, 628.1697, 696.6018, 723.4008, 758.9648, 817.8056, 861.1866, 909.2269, 964.6567, 998.4836, 999.2159, 1012.8382, 1018.1797, 1046.8954, 1051.3401, 1060.7743, 1106.1492, 1125.4608, 1181.2133, 1198.0471, 1278.1377, 1342.5848, 1361.5002, 1479.8149, 1524.6613, 1621.7798, 1641.3918, 1709.0926, 2194.1721, 2305.1575, 2344.6395, 3189.5358, 3197.8549, 3208.501, 3218.4881, 3220.8821]

Benzaldehyde (1)

C	-1.339662	-1.329562	-0.000065
C	0.035520	-1.112295	-0.000082
C	0.537162	0.202101	-0.000131
C	-0.351124	1.290288	-0.000127
C	-1.729543	1.069917	0.000105
C	-2.222073	-0.239104	0.000125
H	-1.730155	-2.342556	-0.000133
H	0.731813	-1.944858	-0.000035
H	0.041210	2.304090	-0.000144
H	-2.415714	1.911013	0.000149
H	-3.294101	-0.412764	0.000168
C	1.987969	0.467091	-0.000010
O	2.861224	-0.393063	0.000153
H	2.267668	1.538955	-0.000111

b3lyp:
Energy+ZPE (kcal/mol): -216801.41334524498

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -216602.94793627

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -216599.15840941903

Frequencies: [115.5773, 217.0947, 236.965, 415.9767, 443.4975, 459.6588, 625.9681, 655.9499, 693.0092, 760.2114, 836.1371, 863.0135, 948.0033, 999.5417, 1011.8453, 1019.4317, 1038.1226, 1041.266, 1103.0574, 1182.6425, 1188.3492, 1230.1089, 1338.0561, 1364.6389, 1432.3603, 1486.9721, 1524.3676, 1624.0882, 1641.7776, 1732.2832, 2956.086, 3186.3284, 3193.4535, 3202.8362, 3211.5391, 3217.0478]

Deuterated Benzaldehyde (1)

C	-1.339662	-1.329562	-0.000065
C	0.035520	-1.112295	-0.000082
C	0.537162	0.202101	-0.000131

C	-0.351124	1.290288	-0.000127
C	-1.729543	1.069917	0.000105
C	-2.222073	-0.239104	0.000125
H	-1.730155	-2.342556	-0.000133
H	0.731813	-1.944858	-0.000035
H	0.041210	2.304090	-0.000144
H	-2.415714	1.911013	0.000149
H	-3.294101	-0.412764	0.000168
C	1.987969	0.467091	-0.000010
O	2.861224	-0.393063	0.000153
H	2.267668	1.538955	-0.000111

b3lyp:
Energy+ZPE (kcal/mol): -216801.41334524498

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -216602.94793627

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -216599.15840941903

Frequencies: [115.5773, 217.0947, 236.965, 415.9767, 443.4975, 459.6588, 625.9681, 655.9499, 693.0092, 760.2114, 836.1371, 863.0135, 948.0033, 999.5417, 1011.8453, 1019.4317, 1038.1226, 1041.266, 1103.0574, 1182.6425, 1188.3492, 1230.1089, 1338.0561, 1364.6389, 1432.3603, 1486.9721, 1524.3676, 1624.0882, 1641.7776, 1732.2832, 2956.086, 3186.3284, 3193.4535, 3202.8362, 3211.5391, 3217.0478]

Enolate (2^-)

C	0.270246	0.006704	-0.010173
C	-0.463951	-1.181748	0.149212
C	-1.861915	-1.177173	0.173549
C	-2.565221	0.022453	0.021130
C	-1.851025	1.213675	-0.155214
C	-0.453374	1.203720	-0.170503
C	1.790575	-0.063555	-0.024590
C	2.504663	1.065350	0.330062
O	2.304633	-1.207238	-0.353324
H	2.022932	1.986522	0.638862
H	0.086133	-2.111678	0.251846
H	-2.402725	-2.110831	0.307872
H	-2.383624	2.151726	-0.290638
H	0.080231	2.136191	-0.327049
H	3.591755	1.039965	0.333819
H	-3.651757	0.029462	0.031041

b3lyp:
Energy+ZPE (kcal/mol): -241150.752376284

b2plypd (solvent=acetonitrile):

Energy+ZPE (kcal/mol): -240923.64682904

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -240927.752620427

Frequencies: [49.5636, 152.5843, 224.9719, 372.5456, 405.8526, 418.834, 495.8698, 587.6173, 599.3381, 614.0413, 630.3182, 703.9318, 716.6902, 748.5321, 791.7948, 863.0756, 935.5395, 990.3151, 1001.2937, 1008.4726, 1015.5324, 1043.0131, 1091.2435, 1124.4768, 1170.7738, 1188.5104, 1315.9918, 1321.7343, 1349.2317, 1424.9125, 1470.0092, 1513.2667, 1556.5522, 1618.977, 1636.2349, 3143.6361, 3170.2647, 3177.4895, 3192.8483, 3200.4321, 3209.3275, 3233.1335]

Deuterated Enolate (2^-)

C	0.270250	0.006701	-0.010171
C	-0.463949	-1.181749	0.149209
C	-1.861919	-1.177170	0.173549
C	-2.565220	0.022449	0.021129
C	-1.851030	1.213680	-0.155211
C	-0.453370	1.203721	-0.170501
C	1.790580	-0.063558	-0.024591
C	2.504660	1.065352	0.330059
O	2.304631	-1.207238	-0.353321
H(Iso=2)	2.022929	1.986522	0.638859
H	0.086132	-2.111679	0.251849
H	-2.402728	-2.110831	0.307869
H	-2.383621	2.151729	-0.290641
H	0.080229	2.136191	-0.327051
H(Iso=2)	3.591760	1.039963	0.333819
H	-3.651760	0.029459	0.031039

b3lyp:
Energy+ZPE (kcal/mol): -241154.556335842

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -240927.442003472

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -240931.58983796198

Frequencies: [48.8224, 148.8682, 216.692, 353.5042, 385.4332, 418.0659, 445.2728, 452.8454, 508.1069, 565.3185, 630.1892, 689.5484, 709.7961, 721.2531, 790.7394, 862.6305, 869.1102, 935.8169, 990.2451, 1001.3155, 1008.983, 1017.587, 1045.3628, 1090.7091, 1158.0289, 1171.3082, 1188.5852, 1319.7861, 1331.7984, 1349.8396, 1460.1215, 1505.6816, 1525.5886, 1617.9975, 1636.2048, 2289.2537, 2406.5531, 3170.2664, 3177.5193, 3192.9449, 3200.6747, 3209.3189]

Water

O	0.000000	0.000000	0.117690
H(Iso=2)	0.000000	0.766980	-0.470760

H(Iso=2)	0.000000	-0.766980	-0.470760

b3lyp:
Energy+ZPE (kcal/mol): -47958.322863589994

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -47924.264812615

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -47926.494352092

Frequencies: [1175.6832, 2738.3113, 2860.0561]

Deuterated Water

O	0.000000	0.000000	0.117690
H(Iso=2)	0.000000	0.766980	-0.470760
H(Iso=2)	0.000000	-0.766980	-0.470760

Hidroxide

O	0.000000	0.000000	0.107497
H	0.000000	0.000000	-0.859975

b3lyp:
Energy+ZPE (kcal/mol): -47642.414752702

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -47603.203597819

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -47621.614084370005

Frequencies: [3806.9213]

Step 2 Product (3^-)

C	2.443028	0.362494	-0.149505
C	3.710742	0.971461	-0.177350
C	4.867758	0.195675	-0.236625
C	4.772837	-1.202115	-0.251127
C	3.517150	-1.816137	-0.206583
C	2.355605	-1.039669	-0.166509
C	1.219562	1.225532	-0.091221
C	-0.123557	0.668853	-0.465987
O	1.321794	2.406092	0.271921
H	-0.046824	-0.187204	-1.141788
H	3.772288	2.054784	-0.158348
H	5.841827	0.675292	-0.270379
H	5.673800	-1.807606	-0.295522
H	3.442140	-2.899891	-0.203140
H	1.379637	-1.506997	-0.090014

H	-0.667416	1.473242	-0.970557
C	-4.245226	-1.493420	-0.330556
C	-2.936881	-1.296319	0.127673
C	-2.423671	-0.006824	0.315987
C	-3.264333	1.085657	0.047624
C	-4.573968	0.898697	-0.405230
C	-5.070481	-0.396407	-0.600367
H	-4.623200	-2.503455	-0.471038
H	-2.293830	-2.139315	0.363203
H	-2.890773	2.097089	0.201256
H	-5.208387	1.759838	-0.600800
H	-6.088369	-0.546395	-0.950218
C	-0.973410	0.195405	0.819702
O	-0.438203	-0.869517	1.447975
H	-1.010547	1.120723	1.448622

b3lyp:
Energy+ZPE (kcal/mol): -457951.764743278

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457531.81313015404

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457539.27421216405

Frequencies: [27.9684, 30.8071, 41.6003, 60.8347, 90.1171, 142.9861, 171.125, 201.532, 241.5063, 254.8542, 359.4068, 385.5729, 414.5093, 418.0256, 419.51, 474.9829, 501.0629, 514.4862, 606.4133, 628.0713, 630.1103, 635.6075, 684.7758, 697.2644, 712.8978, 745.8659, 756.8328, 780.1332, 824.5178, 859.9282, 862.8519, 868.2826, 926.1514, 948.348, 967.1938, 988.3183, 993.375, 1001.2555, 1009.6566, 1009.926, 1014.5304, 1023.4267, 1042.8803, 1050.3818, 1083.9974, 1103.8738, 1138.7352, 1159.977, 1170.8285, 1178.194, 1184.9463, 1194.7177, 1202.1655, 1251.347, 1273.0497, 1298.3587, 1320.3697, 1343.1821, 1349.4248, 1360.6761, 1379.3554, 1472.8962, 1475.4208, 1481.8899, 1515.997, 1525.0319, 1617.0633, 1621.7589, 1636.2123, 1639.1755, 1669.8547, 2749.461, 3065.2902, 3124.5836, 3153.2693, 3168.7198, 3177.7749, 3181.219, 3190.5869, 3193.6568, 3201.4918, 3201.8488, 3211.1347, 3213.1723]

Deuterated Step 2 Product (3^-)

C	2.443030	0.362492	-0.149509
C	3.710739	0.971462	-0.177349
C	4.867760	0.195683	-0.236629
C	4.772840	-1.202117	-0.251129
C	3.517150	-1.816138	-0.206579
C	2.355610	-1.039668	-0.166509
C	1.219559	1.225531	-0.091219
C	-0.123561	0.668851	-0.465989
O	1.321789	2.406091	0.271921
H(Iso=2)	-0.046820	-0.187199	-1.141789
H	3.772289	2.054782	-0.158349
H	5.841829	0.675293	-0.270379

H	5.673800	-1.807607	-0.295519
H	3.442141	-2.899888	-0.203139
H	1.379640	-1.506999	-0.090009
H(Iso=2)	-0.667421	1.473240	-0.970559
C	-4.245230	-1.493421	-0.330559
C	-2.936880	-1.296321	0.127671
C	-2.423670	-0.006820	0.315991
C	-3.264331	1.085659	0.047621
C	-4.573971	0.898699	-0.405229
C	-5.070480	-0.396412	-0.600369
H	-4.623199	-2.503461	-0.471039
H	-2.293829	-2.139310	0.363201
H	-2.890771	2.097089	0.201261
H	-5.208391	1.759838	-0.600799
H	-6.088370	-0.546402	-0.950219
C	-0.973410	0.195410	0.819701
O	-0.438200	-0.869520	1.447981
H	-1.010551	1.120720	1.448621

b3lyp:
Energy+ZPE (kcal/mol): -457955.94897329

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457535.981044932

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457543.466599793

Frequencies: [27.9841, 30.683, 41.5571, 59.5615, 89.472, 142.5083, 167.6137, 200.6714, 235.4267, 253.9963, 352.4338, 359.0638, 411.8122, 415.3474, 419.1692, 452.6195, 474.3627, 508.9199, 579.8905, 617.5966, 628.0877, 630.1918, 680.1763, 696.5706, 712.071, 726.2466, 737.7199, 766.6157, 780.8868, 845.5509, 857.4612, 860.1126, 863.9263, 894.3169, 937.1857, 947.7862, 976.2073, 988.7408, 993.5349, 1001.2216, 1009.6362, 1009.8111, 1014.6188, 1018.6062, 1042.9061, 1050.1815, 1083.9766, 1104.8912, 1129.2318, 1157.1274, 1170.3653, 1178.1453, 1183.1024, 1198.1707, 1200.5991, 1261.723, 1283.614, 1318.4117, 1344.2586, 1349.2132, 1360.9794, 1376.5142, 1475.3106, 1478.0194, 1515.9417, 1523.6973, 1616.5183, 1621.7419, 1636.1332, 1638.6804, 1666.4726, 2227.9051, 2319.064, 2749.7962, 3153.2485, 3168.7045, 3177.7769, 3181.2526, 3190.6202, 3193.6556, 3201.5129, 3201.8868, 3211.0808, 3213.1923]

Step 2 Product (3^-) complex

C	3.01043600	1.05222800	0.05794700
C	2.47429900	-0.22753800	0.25559100
C	3.28742800	-1.33724100	-0.02837600
C	4.59284500	-1.17794800	-0.50245400
C	5.11384400	0.10621900	-0.70261300

C	4.31612800	1.21957600	-0.41944000
H	2.39924500	1.91745600	0.29236500
H	2.89518200	-2.34041200	0.13056100
H	5.20485200	-2.05244600	-0.70884100
H	6.12913200	0.23551300	-1.06759200
H	4.71207300	2.22165500	-0.56556600
C	-1.21004200	-1.34715900	-0.01990400
C	-2.47927100	-0.56403200	-0.18208400
C	-3.70187100	-1.20311000	0.09950500
C	-2.49803200	0.77619000	-0.60482800
C	-4.91008700	-0.52387200	-0.04093400
H	-3.68501100	-2.23702600	0.42717600
C	-3.70995100	1.45955000	-0.73915000
H	-1.57182200	1.30073100	-0.80654900
C	-4.91709600	0.81223100	-0.46199900
H	-5.84563800	-1.03114500	0.17609300
H	-3.70935400	2.49709600	-1.06007800
H	-5.85808900	1.34355400	-0.57218400
O	-1.25340400	-2.47473600	0.48471300
C	0.12346900	-0.79574000	-0.46566900
H	0.60854700	-1.59308100	-1.03945900
H	0.03284700	0.08173800	-1.10892500
C	1.03616300	-0.42217600	0.77594700
H	1.06274300	-1.35429600	1.37977000
O	0.53930000	0.62886600	1.49930000
O	0.08926700	2.95873100	0.59327700
H	-0.81721900	3.15907300	0.85694400
H	0.27163800	1.98562700	0.91873000

b3lyp:
Energy+ZPE (kcal/mol): -505905.48482835

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -504909.4121948070

b2plypd (solvent=water):

Energy+ZPE (kcal/mol): -504915.92839259

Frequencies: [21.9771, 25.6170, 31.9698,53.2604, 79.0901,81.0887, 91.4717, 144.7616, 173.0824, 191.3640, 205.1805, 229.5740, 255.5640, 308.3324,372.0134, 383.0380, 416.3139,417.5401, 431.7556, 477.7988, 485.7139, 528.2743, 596.0535, 613.4848, 628.3963, 629.7572,644.5547, 689.5027, 701.0059, 712.5981, 751.3244, 761.7590,783.3380, 861.1818, 862.5275, 865.1704, 879.7836, 925.2635, 959.4596, 981.7884, 988.1402, 1000.9178, 1002.3314, 1009.6938, 1012.2386, 1013.3395, 1016.4047, 1045.7597, 1048.1966, 1090.4273, 1103.6211, 1123.9884, 1136.0274, 1173.3808, 1174.6632, 1178.6173, 1191.8032, 1199.2832, 1206.9501, 1254.2665, 1286.4077, 1307.1205, 1326.7036, 1342.1503, 1354.3074, 1360.0738, 1381.0231, 1473.5210, 1477.0698, 1482.3413, 1521.5902, 1525.5404, 1619.2552, 1622.8351, 1638.9260, 1639.7426, 1683.9702, 1684.2995, 2362.3916, 2859.2152, 3062.1865, 3129.5025, 3157.1686, 3171.8214, 3180.6820, 3185.2507, 3194.6462, 3196.3074, 3205.7970, 3214.9235, 3217.9336, 3229.9512, 3861.0006

Deuterated Step 2 Product (3^-) complex

C	3.01043600	1.05222800	0.05794700
C	2.47429900	-0.22753800	0.25559100
C	3.28742800	-1.33724100	-0.02837600
C	4.59284500	-1.17794800	-0.50245400
C	5.11384400	0.10621900	-0.70261300
C	4.31612800	1.21957600	-0.41944000
H	2.39924500	1.91745600	0.29236500
H	2.89518200	-2.34041200	0.13056100
H	5.20485200	-2.05244600	-0.70884100
H	6.12913200	0.23551300	-1.06759200
H	4.71207300	2.22165500	-0.56556600
C	-1.21004200	-1.34715900	-0.01990400
C	-2.47927100	-0.56403200	-0.18208400
C	-3.70187100	-1.20311000	0.09950500
C	-2.49803200	0.77619000	-0.60482800
C	-4.91008700	-0.52387200	-0.04093400
H	-3.68501100	-2.23702600	0.42717600
C	-3.70995100	1.45955000	-0.73915000
H	-1.57182200	1.30073100	-0.80654900
C	-4.91709600	0.81223100	-0.46199900
H	-5.84563800	-1.03114500	0.17609300
H	-3.70935400	2.49709600	-1.06007800
H	-5.85808900	1.34355400	-0.57218400
O	-1.25340400	-2.47473600	0.48471300
C	0.12346900	-0.79574000	-0.46566900
H(Iso=2)	0.60854700	-1.59308100	-1.03945900
H(Iso=2)	0.03284700	0.08173800	-1.10892500
C	1.03616300	-0.42217600	0.77594700
H	1.06274300	-1.35429600	1.37977000
O	0.53930000	0.62886600	1.49930000
O	0.08926700	2.95873100	0.59327700
H(Iso=2)	-0.81721900	3.15907300	0.85694400
H(Iso=2)	0.27163800	1.98562700	0.91873000

b3lyp:
Energy+ZPE (kcal/mol): -505924.185851571

b2plypd (solvent=water):

Energy+ZPE (kcal/mol): -504923.981215587

Frequencies: [21.793125.4481,31.5296, 52.1450,78.2297,78.5509, 89.9499,140.8270,148.5187, 172.6066, 192.3305,223.4798, 249.7971, 294.1138,354.8621, 366.4685, 415.9359, 417.4012, 422.5117, 440.9911, 454.3083, 474.4941, 519.1985, 576.7776, 619.6171, 628.2822, 629.9219,

685.8885, 698.9490, 712.1122, 737.8003, 741.3545, 767.4477, 786.2341, 819.1336, 853.9644, 861.9950, 866.3300, 869.9764, 909.1743,950.2068,956.9175, 987.7633,991.2115,1001.2943, 1002.0565, 1009.7218, 1012.7489, 1016.4589, 1031.5047, 1045.7412, 1048.9231, 1090.3702, 1105.3866, 1127.6990, 1147.1131, 1173.2145, 1178.6490, 1182.3067, 1197.2305, 1201.1184, 1222.6824,1274.0079, 1282.2810, 1323.3169, 1342.6117, 1354.8667, 1360.3369, 1376.5573, 1476.7853, 1477.5853, 1521.9347, 1523.5643, 1619.0431, 1623.1327, 1638.6869, 1639.7174, 1680.7894, 1748.6275, 2228.4736, 2319.7345, 2809.4522, 2858.4974, 3157.1542, 3171.8167, 3180.6782, 3185.2455, 3194.6321, 3196.3023, 3205.7797, 3214.8989, 3217.9334, 3229.5092]

Step 3 Product (3)

C	3.321080	-0.058990	-1.130999
C	2.563101	0.283772	-0.004475
C	3.029562	-0.102601	1.262321
C	4.217721	-0.823518	1.399786
C	4.964346	-1.168014	0.267241
C	4.512796	-0.781154	-0.997006
H	2.997395	0.246606	-2.121225
H	2.461751	0.168121	2.149751
H	4.564026	-1.108757	2.389124
H	5.890612	-1.725435	0.371309
H	5.087890	-1.036060	-1.882671
C	-1.274608	0.814903	0.327771
C	-2.563546	0.078778	0.128814
C	-2.610438	-1.282293	-0.221242
C	-3.770659	0.776368	0.318903
C	-3.838170	-1.930371	-0.373709
H	-1.697514	-1.848843	-0.366580
C	-4.994785	0.131369	0.157209
H	-3.730509	1.825672	0.590720
C	-5.030982	-1.225433	-0.188082
H	-3.862115	-2.983102	-0.637910
H	-5.919931	0.681458	0.300433
H	-5.984812	-1.729786	-0.311628
O	-1.273148	1.960765	0.769809
C	0.038678	0.100799	0.016074
H	0.213027	-0.619599	0.826418
H	-0.053171	-0.497712	-0.897937
C	1.244896	1.045620	-0.108587
H	1.197627	1.769247	0.709521
O	1.147140	1.843323	-1.293146
H	0.989828	1.270066	-2.056742

b3lyp:
Energy+ZPE (kcal/mol): -458258.225706171

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457844.799559138

b2plypd (solvent=water):

Energy+ZPE (kcal/mol): -457839.861063308

Frequencies: [21.0812, 23.3067, 31.488, 67.8523, 80.9492, 146.1046, 153.9793, 199.4998, 236.898, 255.263, 328.0328, 334.6414, 385.4723, 410.7608, 413.8265, 423.922, 461.7785, 488.2046, 563.1755, 595.1016, 605.0933, 627.8092, 630.7501, 673.5816, 694.9165, 710.6036, 761.7374, 767.4815, 773.4409, 856.1657, 860.012, 876.0003, 894.2798, 928.8606, 953.6601, 986.066, 989.4476, 998.8455, 1005.7559, 1011.4152, 1012.4372, 1017.7393, 1025.9364, 1048.5419, 1051.8196, 1083.123, 1106.6564, 1109.9719, 1171.9462, 1179.0638, 1180.5241, 1198.57, 1204.1249, 1208.5203, 1223.7112, 1288.7611, 1304.4736, 1340.1922, 1346.0286, 1360.9117, 1361.0718, 1390.2969, 1417.6324, 1454.5909, 1479.6679, 1481.3918, 1525.2288, 1530.2158, 1621.8855, 1628.6038, 1640.9509, 1648.7459, 1720.8687, 3043.7227, 3083.3643, 3103.0963, 3171.8342, 3183.0293, 3189.9722, 3191.6885, 3199.2769, 3199.5406, 3208.3386, 3208.641, 3219.1698, 3221.6375, 3804.0373]

Deuterated Step 3 Product (3)

C	-3.321080	-0.058990	1.130999
C	-2.563101	0.283772	0.004475
C	-3.029562	-0.102601	-1.262321
C	-4.217721	-0.823518	-1.399786
C	-4.964346	-1.168014	-0.267241
C	-4.512796	-0.781154	0.997006
H	-2.997395	0.246606	2.121225
H	-2.461751	0.168121	-2.149751
H	-4.564026	-1.108757	-2.389124
H	-5.890612	-1.725435	-0.371309
H	-5.087890	-1.036060	1.882671
C	1.274608	0.814903	-0.327771
C	2.563546	0.078778	-0.128814
C	2.610438	-1.282293	0.221242
C	3.770659	0.776368	-0.318903
C	3.838170	-1.930371	0.373709
H	1.697514	-1.848843	0.366580
C	4.994785	0.131369	-0.157209
H	3.730509	1.825672	-0.590720
C	5.030982	-1.225433	0.188082
H	3.862115	-2.983102	0.637910
H	5.919931	0.681458	-0.300433
H	5.984812	-1.729786	0.311628
O	1.273148	1.960765	-0.769809
C	-0.038678	0.100799	-0.016074
H(Iso=2)	-0.213027	-0.619599	-0.826418
H(Iso=2)	0.053171	-0.497712	0.897937
C	-1.244896	1.045620	0.108587
H	-1.197627	1.769247	-0.709521
O	-1.147140	1.843323	1.293146
H(Iso=2)	-0.989828	1.270066	2.056742

b3lyp:
Energy+ZPE (kcal/mol): -458264.460635595

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457850.979895279

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457846.10415034904

Frequencies: [21.0543, 23.0691, 30.9866, 65.383, 78.2538, 143.4665, 153.1397, 197.6788, 226.1859, 239.2818, 251.192, 317.7841, 381.1676, 403.5967, 411.6574, 413.8039, 445.9273, 466.0114, 545.1914, 552.5851, 593.885, 627.7711, 630.4296, 669.2202, 694.3523, 710.4902, 746.755, 753.9067, 760.7737, 787.3815, 837.0462, 856.4154, 860.0195, 880.9954, 917.3563, 928.5485, 949.071, 964.2145, 986.1206, 999.0152, 1005.6537, 1011.3598, 1012.4649, 1018.2115, 1038.9664, 1047.1709, 1050.8007, 1077.0961, 1082.7567, 1107.4392, 1120.9712, 1151.9928, 1178.9573, 1181.1634, 1200.0097, 1203.7656, 1218.455, 1275.6416, 1312.7589, 1340.4162, 1344.5705, 1360.9462, 1361.651, 1395.2392, 1479.4145, 1481.1512, 1524.3479, 1530.089, 1621.732, 1628.5498, 1640.7554, 1648.7034, 1718.4925, 2216.5643, 2284.1901, 2769.2972, 3101.3082, 3171.8322, 3183.0357, 3189.971, 3191.692, 3199.2687, 3199.5501, 3208.3416, 3208.6253, 3219.1498, 3221.5701]

Step 3 Product (3) complex

C	2.91299100	1.04117200	-0.17439400
C	2.48353600	-0.23148600	0.23451900
C	3.38593400	-1.30248400	0.15160800
C	4.68519500	-1.11568700	-0.33276800
C	5.10278800	0.15483200	-0.74158900
C	4.21139000	1.23082700	-0.65878700
H	2.22735500	1.88105600	-0.10027300
H	3.07114300	-2.29334600	0.47298000
H	5.37004300	-1.95808500	-0.38352000
H	6.11192900	0.30600100	-1.11487100
H	4.52932600	2.22265800	-0.97026200
C	-1.22844300	-1.29306800	-0.03703900
C	-2.50712600	-0.52845800	-0.17232600
C	-3.72094300	-1.24163000	-0.16700800
C	-2.53205500	0.87272300	-0.28897900
C	-4.93630000	-0.57162500	-0.28964800
H	-3.69330300	-2.32241400	-0.07470900
C	-3.75548800	1.54154900	-0.39377400
H	-1.60923400	1.44926000	-0.25473400
C	-4.95561000	0.82491900	-0.40201300
H	-5.86671400	-1.13189000	-0.29772900
H	-3.76952600	2.62515000	-0.46869900
H	-5.90248800	1.34934500	-0.49466900
O	-1.24348800	-2.44821600	0.39635700
C	0.09598000	-0.68237300	-0.46287800
H	0.55059300	-1.40510200	-1.15046700
H	-0.02782500	0.26117200	-0.99734400
C	1.06033600	-0.46729400	0.74652700
H	1.07334400	-1.41572100	1.30255900

O	0.59495200	0.53050000	1.61652400
O	0.17701800	2.71303900	0.52799400
H	-0.51090400	3.18683400	1.01461100
H	0.40529000	1.49100400	1.12141400

b3lyp:
Energy+ZPE (kcal/mol): -505904.80398109

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -504908.1860861470

b2plypd (solvent=water): -504914.53158266

Frequencies : [21.7931, 25.4481, 31.5296, 52.1450, 78.2297, 78.5509, 89.9499, 140.8270,148.5187, 172.6066, 192.3305, 223.4798, 249.7971, 294.1138, 354.8621, 366.4685, 415.9359, 417.4012, 422.5117, 440.9911, 454.3083, 474.4941 ,519.1985, 576.7776, 619.6171, 628.2822,629.9219, 685.8885, 698.9490,712.1122, 737.8003, 741.3545, 767.4477, 786.2341, 819.1336,853.9644, 861.9950, 866.3300, 869.9764, 909.1743, 950.2068, 956.9175, 987.7633, 991.2115, 1001.2943, 1002.0565, 1009.7218, 1012.7489, 1016.4589, 1031.5047, 1045.7412, 1048.9231, 1090.3702, 1105.3866, 1127.6990, 1147.1131, 1173.2145, 1178.6490,1182.3067, 1197.2305, 1201.1184, 1222.6824, 1274.0079, 1282.2810,1323.3169,1342.6117, 1354.8667, 1360.3369, 1376.5573, 1476.7853, 1477.5853, 1521.9347, 1523.5643, 1619.0431, 1623.1327, 1638.6869, 1639.7174, 1680.7894, 1748.6275, 2228.4736, 2319.7345, 2809.4522, 2858.4974, 3157.1542, 3171.8167, 3180.6782,3185.2455, 3194.6321, 3196.3023, 3205.7797, 3214.8989, 3217.9334, 3229.5092

Deuterated Step 3 Product (3) complex

C	2.91299100	1.04117200	-0.17439400
C	2.48353600	-0.23148600	0.23451900
C	3.38593400	-1.30248400	0.15160800
C	4.68519500	-1.11568700	-0.33276800
C	5.10278800	0.15483200	-0.74158900
C	4.21139000	1.23082700	-0.65878700
H	2.22735500	1.88105600	-0.10027300
H	3.07114300	-2.29334600	0.47298000
H	5.37004300	-1.95808500	-0.38352000
H	6.11192900	0.30600100	-1.11487100
H	4.52932600	2.22265800	-0.97026200
C	-1.22844300	-1.29306800	-0.03703900
C	-2.50712600	-0.52845800	-0.17232600
C	-3.72094300	-1.24163000	-0.16700800
C	-2.53205500	0.87272300	-0.28897900
C	-4.93630000	-0.57162500	-0.28964800
H	-3.69330300	-2.32241400	-0.07470900
C	-3.75548800	1.54154900	-0.39377400
H	-1.60923400	1.44926000	-0.25473400
C	-4.95561000	0.82491900	-0.40201300
H	-5.86671400	-1.13189000	-0.29772900
H	-3.76952600	2.62515000	-0.46869900
H	-5.90248800	1.34934500	-0.49466900
O	-1.24348800	-2.44821600	0.39635700

C	0.09598000	-0.68237300	-0.46287800
H(Iso=2)	0.55059300	-1.40510200	-1.15046700
H(Iso=2)	-0.02782500	0.26117200	-0.99734400
C	1.06033600	-0.46729400	0.74652700
H	1.07334400	-1.41572100	1.30255900
O	0.59495200	0.53050000	1.61652400
O	0.17701800	2.71303900	0.52799400
H(Iso=2)	-0.51090400	3.18683400	1.01461100
H(Iso=2)	0.40529000	1.49100400	1.12141400

b3lyp:
Energy+ZPE (kcal/mol): -505912.089360578

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -505078.504076920

Frequencies : [25.7065, 33.4205, 47.1475, 69.9755, 75.2750, 90.8714, 113.0441, 140.4145, 148.1951, 174.6138, 203.2143, 213.6700, 242.9608, 260.9713, 341.3872, 348.3426, 395.3373, 414.1225, 417.6331, 425.8084, 457.9325,493.8089, 526.5042, 578.2411, 619.5284, 626.8760, 630.1956,689.3605, 705.2264, 714.4389, 744.8893, 752.0126, 774.3457,796.8361, 856.3221, 866.2458, 873.4167, 879.9126, 884.6449, 926.3898, 955.0665, 967.0093, 993.1492, 999.3489, 1004.3030, 1008.9873, 1010.7430, 1010.9484, 1027.7943, 1038.6787, 1048.3495, 1050.6615, 1068.8284, 1095.8041, 1109.4652, 1124.0256, 1134.3925, 1176.2216, 1178.3935, 1201.2603, 1209.1000, 1210.5204, 1241.0152,1280.0285, 1300.4175, 1345.6204, 1351.3015, 1365.6012, 1371.2636,1434.3975, 1477.4605, 1485.7568, 1529.1881, 1529.7595,1620.4904, 1625.1554, 1640.5031, 1645.0105, 1691.2822, 2228.2342, 2324.1233,2783.9690, 3010.2675,3149.4236, 3164.8382, 3174.2776, 3183.8662,3184.3030, 3191.1538,3193.6762, 3199.7426, 3204.2482, 3213.6115]

Step 4 Product (5)

C	2.162972	-0.289305	-0.401042
C	2.724444	0.775573	-1.127276
C	3.699654	1.600068	-0.561484
C	4.150663	1.363423	0.743441
C	3.613121	0.299016	1.472471
C	2.626115	-0.516467	0.904977
C	1.147797	-1.197741	-1.072070
C	-0.130349	-1.332091	-0.546310
O	1.570500	-1.793074	-2.138255
H	2.386549	0.956344	-2.144068
H	4.110083	2.425568	-1.137321
H	4.914246	1.999149	1.182995
H	3.961411	0.100055	2.482686
H	2.218290	-1.343104	1.480079
H	-0.817396	-1.981756	-1.089962
C	-4.456712	-0.202975	-0.055071

C	-3.223479	-0.769322	0.279272
C	-2.059885	0.015354	0.325013
C	-2.169408	1.385307	0.042566
C	-3.401187	1.956831	-0.292539
C	-4.551846	1.163386	-0.344869
H	-5.345748	-0.827575	-0.085840
H	-3.159315	-1.826993	0.515760
H	-1.279962	2.010146	0.082265
H	-3.462268	3.020590	-0.506515
H	-5.510997	1.604085	-0.601871
C	-0.698958	-0.596840	0.622194
O	-0.860924	-1.464884	1.803966
H	-0.022426	0.214681	0.913559
H	-0.266713	-2.212827	1.646904

b3lyp:
Energy+ZPE (kcal/mol): -457952.828371033

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457535.975397351

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457538.977400407

Frequencies: [22.8288, 27.9314, 32.4131, 56.2889, 80.6271, 141.3035, 178.9092, 202.6797, 221.3535, 232.6755, 292.3246, 352.4152, 357.8861, 408.1353, 413.7618, 414.5507, 460.9521, 538.1235, 572.7482, 613.3614, 627.6127, 631.1928, 645.61, 670.2031, 709.5894, 710.5683, 748.916, 760.3549, 781.251, 793.4086, 840.9775, 855.6542, 858.1321, 898.3818, 927.7874, 930.6887, 983.5285, 983.9893, 999.2765, 1000.6894, 1010.1218, 1010.4469, 1043.0775, 1046.4733, 1084.0283, 1094.5544, 1103.9364, 1149.4732, 1174.1511, 1174.6843, 1183.9173, 1194.1514, 1195.2595, 1233.1015, 1275.5582, 1318.0802, 1322.9382, 1341.2325, 1351.555, 1355.5162, 1365.2394, 1409.5898, 1467.7855, 1482.1886, 1516.2524, 1525.4416, 1549.3122, 1616.7365, 1624.1201, 1640.2306, 1644.2474, 3048.4848, 3130.7481, 3168.9897, 3172.3141, 3176.4837, 3178.0959, 3186.1063, 3188.3308, 3192.8568, 3198.0005, 3201.7696, 3204.5432, 3787.8637]

Deuterated Step 4 Product (5)

C	-2.162972	-0.289305	0.401042
C	-2.724444	0.775573	1.127276
C	-3.699654	1.600068	0.561484
C	-4.150663	1.363423	-0.743441
C	-3.613121	0.299016	-1.472471
C	-2.626115	-0.516467	-0.904977
C	-1.147797	-1.197741	1.072070
C	0.130349	-1.332091	0.546310
O	-1.570500	-1.793074	2.138255
H	-2.386549	0.956344	2.144068
H	-4.110083	2.425568	1.137321
H	-4.914246	1.999149	-1.182995
H	-3.961411	0.100055	-2.482686

H	-2.218290	-1.343104	-1.480079
H(Iso=2)	0.817396	-1.981756	1.089962
C	4.456712	-0.202975	0.055071
C	3.223479	-0.769322	-0.279272
C	2.059885	0.015354	-0.325013
C	2.169408	1.385307	-0.042566
C	3.401187	1.956831	0.292539
C	4.551846	1.163386	0.344869
H	5.345748	-0.827575	0.085840
H	3.159315	-1.826993	-0.515760
H	1.279962	2.010146	-0.082265
H	3.462268	3.020590	0.506515
H	5.510997	1.604085	0.601871
C	0.698958	-0.596840	-0.622194
O	0.860924	-1.464884	-1.803966
H	0.022426	0.214681	-0.913559
H(Iso=2)	0.266713	-2.212827	-1.646904

b3lyp:
Energy+ZPE (kcal/mol): -457956.831250944

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457539.99835755

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457543.03236356506

Frequencies: [22.5898, 27.7605, 32.3544, 55.9372, 80.1539, 132.4795, 169.6669, 177.9086, 207.9114, 222.5587, 284.8478, 336.5601, 353.3227, 401.4345, 413.3038, 414.3864, 438.3488, 515.3654, 561.2536, 577.586, 593.5373, 628.8655, 630.2644, 639.5687, 709.5177, 710.5037, 724.3179, 730.9803, 771.4054, 787.4593, 802.3294, 855.3446, 858.014, 887.6621, 916.5286, 929.8142, 940.9363, 983.5192, 983.9246, 996.6332, 999.4218, 1000.9709, 1010.2424, 1010.5789, 1044.8075, 1047.808, 1094.5061, 1096.271, 1113.8804, 1174.1475, 1174.8336, 1193.8659, 1194.1523, 1197.323, 1221.4687, 1301.8831, 1316.4923, 1322.6265, 1351.3691, 1355.4756, 1364.0684, 1396.2917, 1467.0661, 1482.048, 1511.3398, 1525.3029, 1536.9332, 1616.5194, 1624.0949, 1640.1844, 1644.1971, 2306.2578, 2757.3642, 3048.789, 3168.9875, 3172.3153, 3176.4873, 3178.092, 3186.1081, 3188.3289, 3192.8459, 3197.9991, 3201.7693, 3204.5405]

Step 5 Product (4)

C	-2.488077	-0.232859	0.018402
C	-3.661101	-0.941581	-0.299722
C	-4.897428	-0.299074	-0.316984
C	-4.983613	1.062479	-0.000668
C	-3.826963	1.774990	0.328559
C	-2.585270	1.134937	0.331209
C	-1.188421	-0.981662	0.034614
C	0.074755	-0.216588	-0.034685
O	-1.193992	-2.219394	0.088565

H	-3.583925	-1.997236	-0.536860
H	-5.793287	-0.855688	-0.575484
H	-5.947003	1.563721	-0.009829
H	-3.889496	2.828380	0.584135
H	-1.704002	1.705449	0.602397
C	5.019680	-0.556172	0.141904
C	3.723665	-1.071542	0.191850
C	2.601937	-0.236189	0.014130
C	2.821343	1.138735	-0.218156
C	4.114795	1.652143	-0.268520
C	5.219266	0.807959	-0.088318
H	5.870009	-1.216703	0.281861
H	3.570921	-2.132527	0.370129
H	1.979998	1.808928	-0.362291
H	4.265978	2.712203	-0.448990
H	6.225846	1.213356	-0.128254
C	1.270657	-0.837814	0.078253
H	0.016408	0.853328	-0.194777
H	1.249142	-1.914636	0.238230

b3lyp:
Energy+ZPE (kcal/mol): -410307.220852539

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -409922.592976043

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -409915.138796632

Frequencies: [19.2276, 28.0643, 58.8788, 89.4293, 96.6698, 157.0813, 208.744, 221.5746, 275.1118, 305.0284, 410.2312, 413.3462, 414.1866, 448.9164, 494.7367, 530.5577, 574.6747, 628.4161, 629.736, 676.2962, 686.154, 695.4513, 707.8129, 761.3465, 803.9371, 805.0961, 852.885, 858.3383, 887.8428, 903.0356, 939.4674, 950.7396, 990.882, 995.8378, 1009.7098, 1010.1487, 1011.8582, 1015.6508, 1022.3507, 1035.6859, 1047.7699, 1058.6502, 1104.7709, 1109.5912, 1180.4011, 1182.5499, 1197.5297, 1203.917, 1230.5813, 1237.9251, 1320.9247, 1329.0502, 1354.6458, 1359.7308, 1365.3257, 1373.7009, 1477.3679, 1482.3776, 1524.761, 1530.1066, 1605.1928, 1617.9917, 1627.1757, 1641.9453, 1646.647, 1699.4823, 3168.9156, 3185.4887, 3188.7173, 3190.9021, 3197.277, 3199.2566, 3206.2122, 3207.4666, 3213.3287, 3214.8758, 3218.5849, 3228.0841]

Deuterated Step 5 Product (4)

C	2.488077	-0.232859	-0.018402
C	3.661101	-0.941581	0.299722
C	4.897428	-0.299074	0.316984
C	4.983613	1.062479	0.000668
C	3.826963	1.774990	-0.328559
C	2.585270	1.134937	-0.331209
C	1.188421	-0.981662	-0.034614
C	-0.074755	-0.216588	0.034685

O	1.193992	-2.219394	-0.088565
H	3.583925	-1.997236	0.536860
H	5.793287	-0.855688	0.575484
H	5.947003	1.563721	0.009829
H	3.889496	2.828380	-0.584135
H	1.704002	1.705449	-0.602397
C	-5.019680	-0.556172	-0.141904
C	-3.723665	-1.071542	-0.191850
C	-2.601937	-0.236189	-0.014130
C	-2.821343	1.138735	0.218156
C	-4.114795	1.652143	0.268520
C	-5.219266	0.807959	0.088318
H	-5.870009	-1.216703	-0.281861
H	-3.570921	-2.132527	-0.370129
H	-1.979998	1.808928	0.362291
H	-4.265978	2.712203	0.448990
H	-6.225846	1.213356	0.128254
C	-1.270657	-0.837814	-0.078253
H(Iso=2)	-0.016408	0.853328	0.194777
H	-1.249142	-1.914636	-0.238230

b3lyp:
Energy+ZPE (kcal/mol): -410309.26778689696

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -409924.659990689

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -409917.21083135

Frequencies: [19.1731, 28.0381, 58.6458, 88.7162, 90.5527, 155.6853, 203.9857, 221.1052, 272.9523, 303.9372, 410.0431, 412.4498, 413.2409, 445.1335, 489.4218, 516.7687, 572.8792, 628.2173, 629.386, 657.8135, 679.2893, 695.0633, 699.6968, 740.9082, 779.0001, 802.1143, 819.6133, 853.0151, 858.2502, 869.9243, 935.4083, 942.7135, 950.5737, 989.4695, 995.9226, 996.7619, 1010.9433, 1011.8942, 1012.3532, 1015.9512, 1044.7562, 1048.423, 1091.6892, 1107.3316, 1129.8009, 1180.5985, 1182.6802, 1197.8387, 1205.0044, 1230.4277, 1276.6528, 1318.3738, 1341.829, 1357.769, 1360.4722, 1365.4099, 1477.2545, 1480.3312, 1524.154, 1530.0109, 1601.7454, 1617.0311, 1626.4276, 1641.4349, 1645.9206, 1685.1144, 2379.8746, 3169.1001, 3185.4907, 3188.7595, 3190.978, 3197.5128, 3199.3891, 3207.3679, 3207.5394, 3214.2525, 3217.2041, 3219.5339]

Step 1 TS (1‡)

C	0.282968	0.316807	0.138230
C	1.352650	1.153223	-0.223102
C	2.647091	0.646768	-0.352953
C	2.892721	-0.713816	-0.135539
C	1.835191	-1.559547	0.215580
C	0.542418	-1.047677	0.355597
C	-1.100932	0.915589	0.274950

C	-2.147634	0.139029	0.913324
O	-1.305034	2.041839	-0.235351
H	-2.680223	-0.651962	0.023320
H	1.151319	2.205225	-0.395954
H	3.463433	1.310365	-0.624623
H	3.898300	-1.111396	-0.239913
H	2.015886	-2.618383	0.378154
H	-0.268243	-1.717737	0.620347
H	-2.972805	0.773238	1.248180
H	-1.807458	-0.530331	1.707154
O	-3.283654	-1.514455	-0.827739
H	-3.917550	-0.980338	-1.328467

b3lyp:
Energy+ZPE (kcal/mol): -289102.81144503603

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -288840.47879755

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -288846.787145527

Frequencies: [-1067.9733, 35.3298, 61.5606, 92.7688, 108.9658, 158.1046, 232.7049, 373.5346, 412.7867, 420.7216, 452.0484, 493.2675, 543.1141, 621.3338, 629.0564, 664.6779, 690.1337, 700.7946, 755.8724, 781.4636, 860.6715, 936.2472, 969.4716, 992.3418, 1007.7893, 1012.0277, 1036.2209, 1045.0466, 1102.1594, 1116.4701, 1177.0752, 1196.0921, 1295.7745, 1335.1285, 1355.7637, 1380.5984, 1469.8614, 1476.9858, 1522.0512, 1546.002, 1604.8587, 1635.1979, 1646.2343, 3076.105, 3142.7014, 3180.0237, 3188.8229, 3201.3974, 3214.2117, 3218.0703, 3804.6647]

Deuterated Step 1 TS ($1^{\ddagger}$)

C	0.282969	0.316811	0.138230
C	1.352649	1.153221	-0.223100
C	2.647089	0.646771	-0.352950
C	2.892719	-0.713819	-0.135540
C	1.835189	-1.559549	0.215580
C	0.542419	-1.047679	0.355600
C	-1.100931	0.915591	0.274950
C	-2.147631	0.139031	0.913320
O	-1.305031	2.041841	-0.235350
H(Iso=2)	-2.680221	-0.651959	0.023320
H	1.151319	2.205221	-0.395950
H	3.463429	1.310371	-0.624620
H	3.898299	-1.111399	-0.239910
H	2.015889	-2.618379	0.378150
H	-0.268241	-1.717739	0.620350
H(Iso=2)	-2.972811	0.773241	1.248180
H(Iso=2)	-1.807461	-0.530329	1.707150
O	-3.283651	-1.514459	-0.827740
H	-3.917551	-0.980339	-1.328470

b3lyp:
Energy+ZPE (kcal/mol): -289107.91246569704

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -288845.49824204104

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -288851.806590018

Frequencies: [-795.4455, 35.0728, 61.1013, 93.0906, 106.6373, 155.4394, 225.3244, 350.1736, 363.2083, 412.7144, 421.7677, 471.7947, 497.767, 569.024, 593.3686, 628.6531, 632.3972, 696.5668, 724.6217, 752.4722, 853.9183, 860.6932, 872.0928, 946.0369, 987.1588, 992.4315, 1007.6714, 1011.8715, 1024.2595, 1048.4645, 1100.2298, 1134.7646, 1157.7515, 1177.4751, 1196.1375, 1305.8171, 1340.0581, 1355.8945, 1473.886, 1521.163, 1595.046, 1631.5378, 1643.9014, 2235.6137, 2333.9974, 3180.0265, 3188.8283, 3201.3867, 3214.216, 3217.9263, 3804.5623]

Step 2 TS (2‡)

C	2.397041	0.391523	-0.234948
C	3.681674	0.957032	-0.147332
C	4.820647	0.151079	-0.099602
C	4.695415	-1.243160	-0.121906
C	3.422613	-1.819183	-0.192692
C	2.283968	-1.010188	-0.254803
C	1.198112	1.308073	-0.298285
C	-0.049941	0.790929	-0.736502
O	1.347205	2.504501	0.097764
H	-0.077887	-0.129775	-1.310758
H	3.769253	2.038353	-0.120927
H	5.805187	0.607869	-0.043154
H	5.579793	-1.873052	-0.081363
H	3.315070	-2.900617	-0.196253
H	1.302447	-1.469185	-0.281748
H	-0.789158	1.535040	-1.017282
C	-4.134162	-1.456068	-0.566896
C	-2.854673	-1.322406	-0.021604
C	-2.398160	-0.076152	0.433589
C	-3.258014	1.030176	0.346904
C	-4.540314	0.899482	-0.192129
C	-4.982565	-0.345631	-0.655367
H	-4.473086	-2.426803	-0.919300
H	-2.197093	-2.182400	0.063033
H	-2.917185	1.999519	0.704936
H	-5.195060	1.765005	-0.248344
H	-5.979037	-0.450207	-1.075307
C	-1.031871	0.066425	1.056408
O	-0.442855	-0.942674	1.542411
H	-0.876679	1.060051	1.516065

b3lyp:
Energy+ZPE (kcal/mol): -457947.039600508

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457527.647725412

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457529.683364608

Frequencies: [-253.7565, 23.5779, 36.5405, 49.2098, 69.229, 78.6112, 109.2339, 162.3721, 208.9469, 225.9675, 240.4362, 360.6599, 391.8303, 416.6815, 417.1939, 418.8991, 459.3904, 502.1677, 532.0954, 604.6158, 629.0052, 629.367, 645.3931, 691.1129, 705.8623, 708.4312, 743.61, 764.3124, 790.6069, 800.0987, 834.2824, 844.7599, 859.6292, 861.783, 931.5985, 939.7009, 989.7045, 990.7699, 1003.7144, 1004.8858, 1008.916, 1011.3769, 1028.8217, 1042.2235, 1043.8494, 1046.4548, 1092.6631, 1099.2865, 1123.5267, 1173.296, 1175.4237, 1180.1278, 1194.4483, 1201.4727, 1313.0852, 1324.3955, 1332.4538, 1354.586, 1354.7389, 1376.1305, 1461.6912, 1470.8449, 1475.9684, 1514.7294, 1520.3412, 1522.0075, 1564.4462, 1623.6314, 1627.493, 1639.8982, 1640.6079, 2926.4385, 3146.8214, 3167.1571, 3175.4101, 3177.0013, 3183.8813, 3186.2465, 3197.9517, 3198.0988, 3204.1679, 3211.0945, 3220.3777, 3236.555]

Deuterated Step 2 TS (2‡)

C	2.397040	0.391520	-0.234950
C	3.681670	0.957030	-0.147330
C	4.820650	0.151080	-0.099600
C	4.695420	-1.243160	-0.121910
C	3.422610	-1.819180	-0.192690
C	2.283970	-1.010190	-0.254800
C	1.198110	1.308070	-0.298290
C	-0.049940	0.790930	-0.736500
O	1.347210	2.504500	0.097760
H(Iso=2)	-0.077890	-0.129780	-1.310760
H	3.769250	2.038350	-0.120930
H	5.805190	0.607870	-0.043150
H	5.579790	-1.873050	-0.081360
H	3.315070	-2.900620	-0.196250
H	1.302450	-1.469190	-0.281750
H(Iso=2)	-0.789160	1.535040	-1.017280
C	-4.134160	-1.456070	-0.566900
C	-2.854670	-1.322410	-0.021600
C	-2.398160	-0.076150	0.433590
C	-3.258010	1.030180	0.346900
C	-4.540310	0.899480	-0.192130
C	-4.982570	-0.345630	-0.655370
H	-4.473090	-2.426800	-0.919300

H	-2.197090	-2.182400	0.063030
H	-2.917190	1.999520	0.704940
H	-5.195060	1.765010	-0.248340
H	-5.979040	-0.450210	-1.075310
C	-1.031870	0.066430	1.056410
O	-0.442860	-0.942670	1.542410
H	-0.876680	1.060050	1.516070

b3lyp:
Energy+ZPE (kcal/mol): -457951.060050671

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457531.624877454

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457533.686872028

Frequencies: [-252.4725, 23.2753, 36.4151, 49.1469, 68.6622, 78.0657, 108.0854, 160.1156, 208.0841, 225.684, 235.4795, 354.2946, 360.5402, 409.3187, 416.8197, 417.1461, 446.7049, 478.5271, 521.2619, 563.7596, 583.9625, 619.4292, 628.9936, 629.3496, 673.3598, 698.7038, 706.1108, 715.754, 731.9729, 767.8414, 807.1487, 831.2266, 859.1017, 861.5029, 876.8961, 931.3272, 939.6739, 989.6909, 990.6566, 1002.3903, 1003.7439, 1005.8323, 1010.5083, 1011.7927, 1036.6926, 1042.3155, 1048.5405, 1092.6983, 1097.6606, 1160.359, 1173.2838, 1176.0207, 1180.1325, 1194.3036, 1201.4669, 1321.0525, 1324.6948, 1342.6759, 1354.5658, 1355.1168, 1377.1067, 1461.4001, 1470.6925, 1511.9236, 1519.8723, 1521.5979, 1555.8748, 1623.0311, 1627.4746, 1639.883, 1640.5062, 2286.8356, 2409.7418, 2926.4736, 3167.17, 3175.4246, 3177.0342, 3183.855, 3186.2198, 3197.9924, 3198.0927, 3204.197, 3211.1085, 3220.7811]

Step 3 TS (3‡)

C	2.959365	1.046652	-0.016136
C	2.508461	-0.267579	0.185879
C	3.391849	-1.325643	-0.076335
C	4.691505	-1.085163	-0.535372
C	5.129682	0.227493	-0.737983
C	4.258108	1.290630	-0.475020
H	2.289485	1.875030	0.197371
H	3.061258	-2.350089	0.083773
H	5.360852	-1.919768	-0.727046
H	6.139090	0.419981	-1.091011
H	4.591728	2.314346	-0.625472
C	-1.210748	-1.244061	-0.238940
C	-2.483774	-0.458518	-0.282618
C	-3.702361	-1.156978	-0.377299
C	-2.499409	0.946156	-0.219498
C	-4.912456	-0.467842	-0.422068
H	-3.682535	-2.240827	-0.423587
C	-3.717378	1.632352	-0.247185
H	-1.573589	1.506010	-0.104842
C	-4.922061	0.931658	-0.355488

H	-5.846310	-1.015711	-0.508047
H	-3.723661	2.716732	-0.183557
H	-5.864732	1.470665	-0.386984
O	-1.238573	-2.446643	0.036639
C	0.120124	-0.592046	-0.569109
H	0.570321	-1.212520	-1.352896
H	0.006878	0.420110	-0.961228
C	1.081685	-0.558293	0.663773
H	1.087119	-1.580449	1.072533
O	0.624299	0.311503	1.658721
O	0.213715	2.605888	0.921902
H	-0.479681	2.985342	1.477958
H	0.427721	1.378998	1.299923

b3lyp:
Energy+ZPE (kcal/mol): -505916.54655700503

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -505465.442887085

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -505471.75249008

Frequencies: [-373.4915, 22.7726, 39.4815, 43.5581, 58.2599, 79.5195, 102.263, 130.07, 143.0333, 170.0583, 194.2382, 208.4519, 228.1146, 255.7643, 350.544, 375.3838, 413.933, 418.8084, 422.6788, 484.6308, 497.1823, 537.6692, 558.7633, 607.4375, 626.9058, 629.1373, 638.8078, 692.8721, 705.1935, 715.3122, 752.6004, 765.0751, 777.9828, 803.3935, 867.2412, 873.4879, 884.4398, 894.1013, 935.9238, 968.359, 992.8522, 1002.7505, 1006.1922, 1010.3254, 1011.2821, 1014.0206, 1028.6045, 1030.3448, 1050.1483, 1052.1561, 1093.0617, 1105.8152, 1122.2535, 1175.7915, 1177.6651, 1187.9382, 1204.8109, 1207.2227, 1217.7845, 1254.9213, 1274.456, 1289.8274, 1334.112, 1343.5789, 1348.6433, 1366.9171, 1368.5082, 1413.383, 1473.0894, 1481.8602, 1484.0967, 1528.6538, 1531.0197, 1620.3546, 1624.5655, 1640.3697, 1644.3012, 1692.9461, 1699.5024, 2988.0984, 3057.5493, 3135.0923, 3158.379, 3162.1857, 3172.9706, 3182.6278, 3183.6109, 3192.9629, 3193.6747, 3198.958, 3203.7073, 3213.6517, 3828.7053]

Deuterated Step 3 TS (3‡)

C	2.924410	1.045253	-0.156009
C	2.486081	-0.228957	0.238438
C	3.377704	-1.306736	0.128762
C	4.673180	-1.125347	-0.367720
C	5.098782	0.147110	-0.762448
C	4.218936	1.230119	-0.652849
H	2.248108	1.890449	-0.062139
H	3.056931	-2.299435	0.438725
H	5.349082	-1.973519	-0.439081
H	6.104906	0.294154	-1.145439
H	4.542787	2.223532	-0.953166
C	-1.226099	-1.287391	-0.018373
C	-2.506230	-0.527100	-0.169305

C	-3.718959	-1.241824	-0.154092
C	-2.534088	0.871540	-0.312084
C	-4.935321	-0.576539	-0.292363
H	-3.689702	-2.320597	-0.041579
C	-3.758220	1.536340	-0.432985
H	-1.612796	1.449679	-0.285642
C	-4.957078	0.817532	-0.430996
H	-5.864625	-1.138699	-0.292140
H	-3.773867	2.618283	-0.528496
H	-5.904631	1.338430	-0.535678
O	-1.242034	-2.436946	0.430167
C	0.097483	-0.679813	-0.447703
H(Iso=2)	0.549795	-1.404511	-1.134884
H(Iso=2)	-0.026445	0.263183	-0.982912
C	1.064029	-0.458316	0.761626
H	1.080312	-1.409652	1.315359
O	0.603222	0.543827	1.621296
O	0.169079	2.702409	0.559341
H(Iso=2)	-0.525261	3.153404	1.057823
H(Iso=2)	0.395610	1.545758	1.111425

b3lyp:
Energy+ZPE (kcal/mol): -505923.94990818703

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -505472.673045783

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -505478.929938022

Frequencies: [-289.5372, 5.0243, 27.4693, 33.8227, 58.613, 76.6491, 89.5998, 115.5293, 138.9854, 146.3225, 178.7268, 203.7272, 220.8097, 249.3232, 334.8181, 348.5696, 402.2337, 415.3468, 416.9973, 424.0391, 457.399, 494.239, 525.8305, 577.7307, 617.1535, 626.9248, 630.3602, 687.7935, 697.4231, 707.3972, 714.2011, 746.0263, 759.5886, 778.6745, 796.6275, 857.6731, 866.3354, 870.9476, 881.2274, 908.6129, 932.4906, 961.5207, 964.2941, 992.6861, 998.9311, 1005.7605, 1009.3017, 1010.6185, 1010.9209, 1026.7587, 1047.8316, 1050.0235, 1064.5691, 1093.236, 1108.8982, 1125.8952, 1136.8709, 1175.9147, 1178.3282, 1200.2103, 1207.2703, 1209.3582, 1235.6888, 1278.8599, 1297.6641, 1343.0773, 1345.4959, 1364.204, 1368.919, 1413.0706, 1477.2927, 1484.3013, 1528.495, 1528.6847, 1620.3462, 1624.5781, 1640.0227, 1644.1868, 1690.4535, 2227.3207, 2324.1752, 2787.1551, 2991.3026, 3158.6644, 3163.7097, 3174.0017, 3183.6978, 3184.5083, 3193.9207, 3194.2866, 3199.7789, 3204.4483, 3213.8769]

Step 4 TS (4‡)

C	3.294262	0.854949	0.493712
C	2.473213	-0.215401	0.111944
C	2.703587	-0.820843	-1.133821
C	3.717669	-0.364793	-1.980873
C	4.526166	0.709771	-1.592519
C	4.310312	1.316229	-0.350787

H	3.141793	1.319208	1.463141
H	2.082974	-1.659781	-1.441806
H	3.881411	-0.851599	-2.938672
H	5.317929	1.064430	-2.246428
H	4.936203	2.147336	-0.036164
C	-1.163985	-0.857499	0.494455
C	-2.389876	-0.299811	-0.199203
C	-2.568598	1.071691	-0.451431
C	-3.399432	-1.191247	-0.599956
C	-3.722944	1.535938	-1.087897
H	-1.815467	1.785738	-0.136211
C	-4.548324	-0.731354	-1.246125
H	-3.266177	-2.248783	-0.396949
C	-4.715023	0.636257	-1.491433
H	-3.848514	2.600386	-1.265171
H	-5.313941	-1.437170	-1.556249
H	-5.610441	0.997701	-1.989124
O	-1.236268	-2.011652	0.973896
C	0.008100	-0.009806	0.621734
H	0.110259	0.709953	-0.192292
H	-0.225169	0.767704	1.685632
C	1.329663	-0.706182	0.992721
H	1.212021	-1.783872	0.823271
O	1.655176	-0.563509	2.389932
O	-0.170207	1.355825	2.844821
H	0.125307	2.263943	2.684290
H	1.108984	0.183384	2.745023

b3lyp:
Energy+ZPE (kcal/mol): -505906.427346871

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -505455.250258398

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -505458.940011318

Frequencies: [-1226.5306, 24.8472, 29.9495, 38.5829, 49.5591, 73.5364, 97.7564, 136.3383, 171.7147, 203.7381, 219.3382, 243.068, 271.4371, 304.0246, 328.25, 384.7327, 415.0408, 415.7222, 421.9772, 480.3144, 493.7036, 524.5657, 568.7224, 618.6763, 629.3087, 630.2924, 649.3559, 674.2638, 702.9163, 710.7896, 720.8438, 769.507, 789.1293, 790.3967, 796.4442, 858.9539, 862.8055, 873.5224, 922.9314, 935.5965, 953.7433, 985.7356, 994.9055, 997.3905, 1001.4663, 1009.7308, 1010.8135, 1011.7963, 1039.9083, 1047.6698, 1049.781, 1091.3097, 1099.623, 1110.7758, 1175.0642, 1176.5035, 1191.5196, 1195.7608, 1207.0332, 1223.0612, 1267.5641, 1291.5723, 1330.3859, 1337.3897, 1355.0093, 1355.2759, 1394.8057, 1438.0547, 1474.8046, 1479.4841, 1487.0298, 1522.3014, 1524.8331, 1569.1808, 1607.613, 1624.6721, 1635.1187, 1644.0075, 1646.7201, 3030.9165, 3116.6557, 3166.0053, 3175.5466, 3179.2693, 3184.8461, 3187.7019, 3197.0231, 3200.4036, 3203.6604, 3212.1335, 3214.3528, 3292.0315, 3811.6258]

Deuterated Step 4 TS (4‡)

C	-3.325349	0.283315	0.706071
C	-2.439685	-0.029998	-0.334579
C	-2.576750	-1.271865	-0.975314
C	-3.562752	-2.181335	-0.582244
C	-4.436429	-1.860885	0.463306
C	-4.313677	-0.623830	1.104330
H	-3.245131	1.248461	1.196616
H	-1.904969	-1.527385	-1.792169
H	-3.653868	-3.134943	-1.095568
H	-5.206605	-2.563508	0.768948
H	-4.990742	-0.361780	1.913267
C	1.196114	0.557867	-0.807019
C	2.432201	-0.083064	-0.210124
C	2.564899	-0.357091	1.162421
C	3.499233	-0.409545	-1.064124
C	3.730576	-0.942530	1.664006
H	1.765907	-0.098435	1.848819
C	4.660175	-1.004858	-0.567330
H	3.400999	-0.189504	-2.122086
C	4.780676	-1.272519	0.800939
H	3.819467	-1.137444	2.729064
H	5.470996	-1.257960	-1.244849
H	5.685040	-1.730653	1.191262
O	1.292300	1.066917	-1.946656
C	-0.016542	0.603790	-0.009570
H(Iso=2)	-0.105908	-0.230853	0.687935
H(Iso=2)	0.125730	1.660276	0.799386
C	-1.324829	0.920748	-0.755910
H	-1.151956	0.782599	-1.830618
O	-1.730501	2.295257	-0.598852
O	-0.016486	2.801111	1.408399
H	-0.341842	2.604381	2.299027
H(Iso=2)	-1.236790	2.661259	0.178681

b3lyp:
Energy+ZPE (kcal/mol): -505911.86659488303

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -505460.622990456

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -505464.25375753

Frequencies: [-900.9663, 18.7113, 22.8688, 33.3222, 40.2196, 68.6075, 96.8533, 130.3073, 171.7957, 201.6839, 217.8812, 240.5069, 266.8614, 295.9671, 321.2966, 381.3382, 414.4912, 414.6696, 418.9844, 439.7864, 478.7847, 505.6133, 559.6719, 598.5378, 604.6341, 622.4307, 629.3257, 631.7275, 671.0039, 674.8725, 703.4538, 710.3779, 750.5883, 767.947, 788.0223, 820.4987, 858.427, 861.2557, 868.5586, 911.4864, 928.0028, 943.7776, 952.6855, 985.3199, 986.7498, 993.4875, 1000.9146, 1009.1533, 1010.7313, 1011.4967, 1034.8727,

1047.2546, 1048.4349, 1094.6931, 1099.0154, 1117.6396, 1152.9914, 1164.4641, 1173.7427, 1176.9797, 1191.6079, 1195.4445, 1214.6491, 1282.7614, 1326.0812, 1329.9143, 1350.5524, 1354.3924, 1354.8181, 1383.1701, 1474.2123, 1479.4586, 1520.8625, 1524.692, 1597.9382, 1624.2703, 1631.5616, 1642.9094, 1644.8949, 2293.8087, 2405.2582, 3031.4631, 3166.9675, 3176.7843, 3180.1553, 3186.0561, 3188.6089, 3198.6597, 3201.144, 3205.7607, 3212.3403, 3214.5797, 3812.7724]

Step 5 TS (5‡)

C	2.723557	-0.840632	0.748979
C	2.470994	0.087124	-0.280707
C	3.525529	0.926472	-0.688815
C	4.782397	0.852727	-0.085306
C	5.016938	-0.073103	0.936897
C	3.981540	-0.921370	1.347846
H	1.935940	-1.513090	1.074618
H	3.351758	1.642240	-1.488032
H	5.578380	1.514981	-0.414171
H	5.994681	-0.136097	1.405729
H	4.155500	-1.648493	2.136206
C	-1.310761	0.358914	-0.817036
C	-2.567627	0.011064	-0.051205
C	-2.646071	-1.069368	0.845221
C	-3.719775	0.787743	-0.264547
C	-3.840435	-1.360131	1.510668
H	-1.783222	-1.705423	1.011928
C	-4.909551	0.507859	0.408769
H	-3.664197	1.614369	-0.965029
C	-4.974541	-0.569740	1.299801
H	-3.885054	-2.206357	2.190385
H	-5.785981	1.126949	0.238399
H	-5.900930	-0.793442	1.821102
O	-1.432421	1.017318	-1.879062
C	-0.042530	-0.053259	-0.275465
H	-0.035202	-0.599683	0.660103
C	1.147960	0.232452	-0.916092
H	1.106413	0.914607	-1.754909
O	1.542920	-1.236259	-2.553453
H	2.265140	-1.726432	-2.134830

b3lyp:
Energy+ZPE (kcal/mol): -457942.222841424

b2plypd (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457523.128405594

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457528.309119898

Frequencies: [-170.1617, 28.1397, 40.2579, 57.7293, 78.6539, 93.3895, 108.1247, 136.3544, 151.5188, 198.4665, 224.8203, 239.529, 302.1291, 354.87, 409.3138, 414.5869, 416.6806, 464.8149, 514.9792, 537.7737, 543.0412, 593.9886, 629.3966, 631.4632, 675.9672, 692.4225, 701.0008, 710.868, 754.5927, 791.6511, 808.6772, 825.6144, 853.6908, 860.7563, 905.48, 928.6282, 945.1086, 984.9953, 990.2739, 993.1005, 1003.4245, 1009.3332, 1010.3169, 1011.2942, 1043.5027, 1047.3491, 1083.4996, 1098.1914, 1105.2929, 1176.0716, 1177.4125, 1193.3467, 1199.1761, 1220.1645, 1229.5145, 1288.552, 1321.5068, 1335.2436, 1354.7339, 1359.8074, 1373.9142, 1469.8312, 1479.465, 1517.5993, 1525.6058, 1542.2266, 1604.4198, 1621.0884, 1634.0879, 1642.3382, 1644.3026, 3176.8242, 3180.1587, 3182.2921, 3188.2667, 3191.1184, 3198.1557, 3200.0021, 3205.2471, 3207.4064, 3213.1726, 3217.5648, 3237.4577, 3809.4492]

Deuterated Step 5 TS (5‡)

C	2.645258	1.216735	0.280994
C	2.463790	-0.125411	-0.106931
C	3.551776	-0.796666	-0.697527
C	4.772297	-0.151199	-0.905082
C	4.936212	1.182369	-0.515470
C	3.867041	1.861115	0.081741
H	1.830821	1.756545	0.754152
H	3.433086	-1.835282	-0.994946
H	5.595109	-0.689026	-1.367731
H	5.885631	1.686341	-0.671579
H	3.986345	2.894887	0.394093
C	-1.278198	-0.937851	-0.081344
C	-2.580401	-0.168794	-0.086584
C	-2.724390	1.100947	0.500011
C	-3.707165	-0.761537	-0.682610
C	-3.957807	1.758486	0.486138
H	-1.881757	1.574636	0.992408
C	-4.936269	-0.101369	-0.709742
H	-3.600627	-1.746420	-1.125025
C	-5.066487	1.163047	-0.123502
H	-4.052559	2.733782	0.955098
H	-5.792517	-0.571774	-1.185123
H	-6.023423	1.676908	-0.138139
O	-1.331282	-2.185181	-0.213811
C	-0.048059	-0.201013	0.042851
H(Iso=2)	-0.100470	0.877656	0.130287
C	1.180049	-0.834251	0.050572
H	1.195035	-1.886530	-0.200747
O	1.642121	-1.649694	2.079266
H(Iso=2)	2.332715	-1.020369	2.332536

b3lyp:
Energy+ZPE (kcal/mol): -457946.095826972

b2plypd (solvent=acetonitrile):

Energy+ZPE (kcal/mol): -457526.95621049404

b2plypd (solvent=water):
Energy+ZPE (kcal/mol): -457532.194028117

Frequencies: [-188.5667, 29.9552, 30.8769, 56.7653, 58.8997, 80.7421, 101.0042, 104.7915, 147.6501, 194.9722, 221.9072, 231.3404, 299.2328, 325.8663, 392.572, 408.8738, 414.7993, 416.595, 453.4722, 509.4912, 524.9155, 578.8227, 625.7137, 629.4233, 632.6801, 675.6601, 699.4702, 702.7762, 722.8771, 772.9371, 805.4534, 811.4356, 853.0261, 860.1675, 880.1943, 925.4822, 943.1276, 944.5058, 965.7299, 986.4117, 992.9532, 1003.3492, 1008.8159, 1010.8731, 1011.4862, 1045.1638, 1048.3975, 1094.5694, 1101.8825, 1135.2968, 1176.8007, 1177.7636, 1194.9824, 1200.4276, 1220.1989, 1250.1199, 1309.8901, 1334.7715, 1350.7367, 1355.6572, 1360.2727, 1467.9444, 1475.5188, 1516.3162, 1523.137, 1537.3868, 1591.8015, 1621.0467, 1629.5691, 1642.1501, 1643.7754, 2369.8534, 2774.9638, 3177.5594, 3181.0309, 3183.1691, 3189.0844, 3191.9756, 3200.1246, 3201.4445, 3207.4252, 3210.9125, 3214.0479, 3231.6576]

Calculated atomic coordinates (in angstroms), for all optimized structures of base- catalyzed chalcone reaction at X3LYP/6-31+G(3df,3dp) level of theory.

Acetophenone (2)

C	0.208541	-0.065515	0.000004
C	-0.583457	-1.228155	0.000009
C	-1.973161	-1.136469	-0.000016
C	-2.591982	0.119429	-0.000046
C	-1.814913	1.281143	-0.000052
C	-0.422081	1.191147	-0.000026
C	1.694973	-0.194599	0.000038
C	2.547252	1.048159	0.000041
O	2.227055	-1.311573	0.000041
H	2.334492	1.662729	0.882664
H	-0.101547	-2.200382	0.000033
H	-2.575503	-2.040492	-0.000012
H	-2.291989	2.256966	-0.000075
H	0.166478	2.102376	-0.000032
H	2.334498	1.662728	-0.882585
H	3.602288	0.766905	0.000045
H	-3.676194	0.190910	-0.000065

x3lyp:
Energy+ZPE (kcal/mol): -241341.60421856202

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -241413.649154361

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -241409.72722311103

Frequencies: [35.0447, 149.0293, 164.2655, 218.9905, 372.137, 410.3897, 431.4847, 469.3821, 599.2911, 609.6007, 629.5096, 694.7537, 748.8402, 777.5745, 864.3625, 955.8035, 976.3276, 1003.1228, 1015.7742, 1024.1734, 1046.3476, 1053.8452, 1101.8182, 1112.0894, 1180.5584, 1195.6483, 1290.5819, 1345.9569, 1365.0131, 1404.1403, 1472.0943, 1476.4543,

1484.9107, 1532.2448, 1625.5646, 1645.1942, 1676.53, 3064.8294, 3126.1637, 3166.9621, 3201.5499, 3210.2124, 3219.3103, 3228.4978, 3232.2251]

Deuterated Acetophenone (2)

C	0.208541	-0.065515	0.000004
C	-0.583457	-1.228155	0.000009
C	-1.973161	-1.136469	-0.000016
C	-2.591982	0.119429	-0.000046
C	-1.814913	1.281143	-0.000052
C	-0.422081	1.191147	-0.000026
C	1.694973	-0.194599	0.000038
C	2.547252	1.048159	0.000041
O	2.227055	-1.311573	0.000041
H(Iso=2)	2.334492	1.662729	0.882664
H	-0.101547	-2.200382	0.000033
H	-2.575503	-2.040492	-0.000012
H	-2.291989	2.256966	-0.000075
H	0.166478	2.102376	-0.000032
H(Iso=2)	2.334498	1.662728	-0.882585
H(Iso=2)	3.602288	0.766905	0.000045
H	-3.676194	0.190910	-0.000065

x3lyp:
Energy+ZPE (kcal/mol): -241347.63520756102

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -241419.547111452

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -241415.628945256

Frequencies: [33.8464, 117.076, 147.336, 208.5018, 352.4628, 409.4284, 419.2707, 449.27, 544.1849, 559.0205, 629.4435, 694.1778, 728.3109, 763.2094, 826.1038, 864.3222, 916.2801, 969.8817, 1003.0737, 1004.0513, 1015.8158, 1024.8675, 1050.439, 1052.3855, 1063.8245, 1110.0825, 1137.4411, 1180.6379, 1196.211, 1290.3063, 1348.3955, 1365.048, 1484.6198, 1531.7516, 1624.4345, 1644.4829, 1672.4729, 2203.8332, 2313.106, 2348.9488, 3201.5474, 3210.2035, 3219.3001, 3228.4865, 3232.1729]

Benzaldehyde (1)

C	1.341528	-1.328254	-0.000067
C	-0.033526	-1.115871	0.000186
C	-0.537541	0.197714	0.000323
C	0.346964	1.289020	0.000173
C	1.725110	1.072313	-0.000085
C	2.220293	-0.235130	-0.000208
H	1.735317	-2.340520	-0.000167
H	-0.722668	-1.955151	0.000313
H	-0.051419	2.300724	0.000268
H	2.409456	1.915651	-0.000195
H	3.293248	-0.406640	-0.000412
C	-1.980319	0.468147	0.000677
O	-2.862198	-0.392210	-0.000641
H	-2.261413	1.535988	-0.000673

x3lyp:
Energy+ZPE (kcal/mol): -216696.51454824203

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -216756.09715530102

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -216752.443797903

Frequencies: [120.5241, 227.2017, 236.0831, 416.4651, 444.5585, 460.0894, 627.1594, 656.9294, 692.8349, 763.6649, 840.4025, 865.7498, 954.7813, 1003.8314, 1014.6704, 1025.8975, 1044.7363, 1046.8762, 1109.1398, 1182.1585, 1191.3217, 1241.1246, 1348.2391, 1370.8447, 1445.0855, 1493.081, 1532.9609, 1628.7577, 1647.0823, 1695.3746, 3013.7876, 3199.8519, 3205.3263, 3213.9674, 3222.3525, 3227.3936]

Deuterated Benzaldehyde (1)

C	1.341528	-1.328254	-0.000067
C	-0.033526	-1.115871	0.000186
C	-0.537541	0.197714	0.000323
C	0.346964	1.289020	0.000173
C	1.725110	1.072313	-0.000085
C	2.220293	-0.235130	-0.000208
H	1.735317	-2.340520	-0.000167
H	-0.722668	-1.955151	0.000313
H	-0.051419	2.300724	0.000268
H	2.409456	1.915651	-0.000195
H	3.293248	-0.406640	-0.000412
C	-1.980319	0.468147	0.000677
O	-2.862198	-0.392210	-0.000641
H	-2.261413	1.535988	-0.000673

x3lyp:
Energy+ZPE (kcal/mol): -216696.51454824203

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -216756.09715530102

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -216752.443797903

Frequencies: [120.5241, 227.2017, 236.0831, 416.4651, 444.5585, 460.0894, 627.1594, 656.9294, 692.8349, 763.6649, 840.4025, 865.7498, 954.7813, 1003.8314, 1014.6704, 1025.8975, 1044.7363, 1046.8762, 1109.1398, 1182.1585, 1191.3217, 1241.1246, 1348.2391, 1370.8447, 1445.0855, 1493.081, 1532.9609, 1628.7577, 1647.0823, 1695.3746, 3013.7876, 3199.8519, 3205.3263, 3213.9674, 3222.3525, 3227.3936]

Enolate (2^-)

C	0.268438	0.000112	-0.009723
C	-0.466940	-1.183734	0.174128
C	-1.864199	-1.172993	0.196468
C	-2.562171	0.025300	0.019116

C	-1.845648	1.210519	-0.179315
C	-0.448914	1.196663	-0.193506
C	1.779934	-0.052213	-0.021561
C	2.493634	1.047443	0.384102
O	2.319864	-1.186216	-0.415404
H	2.012555	1.953516	0.737990
H	0.065322	-2.120546	0.308128
H	-2.407316	-2.102215	0.350895
H	-2.375152	2.147560	-0.333372
H	0.088040	2.124668	-0.367133
H	3.581811	1.024772	0.380487
H	-3.648979	0.035389	0.027984

x3lyp:
Energy+ZPE (kcal/mol): -241036.763483907

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -241102.27981607

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -241107.111007861

Frequencies: [61.176, 150.0826, 230.2098, 373.5554, 401.6073, 415.2859, 507.4619, 598.2798, 630.036, 633.6042, 647.745, 705.4839, 730.4955, 755.9613, 795.5665, 863.9246, 939.2766, 992.7463, 1006.3286, 1008.3247, 1012.3078, 1049.1259, 1102.4543, 1132.2103, 1175.5302, 1198.6816, 1296.8133, 1336.0175, 1359.2628, 1404.9441, 1478.7445, 1527.3617, 1572.9528, 1627.8027, 1647.306, 3155.6573, 3187.0987, 3194.0403, 3206.3995, 3212.8305, 3217.4509, 3241.9295]

Deuterated Enolate (2^-)

C	0.268398	0.000273	-0.009681
C	-0.466880	-1.183631	0.174188
C	-1.864162	-1.173011	0.196575
C	-2.562249	0.025218	0.019174
C	-1.845811	1.210437	-0.179384
C	-0.449037	1.196703	-0.193618
C	1.780013	-0.052187	-0.021553
C	2.493887	1.047307	0.384289
O	2.319823	-1.186158	-0.415663
H(Iso=2)	2.013043	1.953398	0.738388
H	0.065307	-2.120477	0.308251
H	-2.407194	-2.102279	0.351016
H	-2.375376	2.147435	-0.333522
H	0.087659	2.124807	-0.367435
H(Iso=2)	3.582082	1.024457	0.380633
H	-3.649061	0.035264	0.028040

x3lyp:
Energy+ZPE (kcal/mol): -241040.62705682

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -241106.081265592

M08HX (solvent=water):

Energy+ZPE (kcal/mol): -241110.951362941

Frequencies: [57.6494, 146.4311, 221.7602, 354.7989, 385.9587, 414.7683, 461.3063, 489.0255, 524.7313, 567.5517, 630.8268, 695.3807, 709.6709, 728.1228, 794.4655, 863.1315, 866.8289, 939.2746, 992.7365, 1008.0808, 1012.0113, 1027.8857, 1053.806, 1102.305, 1162.4146, 1175.5941, 1198.7358, 1280.8781, 1335.1838, 1359.4214, 1467.9939, 1510.3033, 1536.1429, 1626.9492, 1647.1852, 2300.1285, 2413.7677, 3187.0851, 3194.062, 3206.5224, 3213.0802, 3217.4655]

Water

O	0.000000	-0.000000	0.119170
H	0.000000	0.767261	-0.476682
H	-0.000000	-0.767261	-0.476682

x3lyp:
Energy+ZPE (kcal/mol): -47933.435229141

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -47940.709940978006

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -47943.134635753995

Frequencies: [1639.9055, 3720.3496, 3815.1606]

Deuterated Water

O	-0.000000	0.000000	0.119170
H(Iso=2)	-0.000000	0.767261	-0.476682
H(Iso=2)	-0.000000	-0.767261	-0.476682

x3lyp:
Energy+ZPE (kcal/mol): -47937.003872824

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -47944.267917008

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -47946.690729257

Frequencies: [1199.4286, 2683.7008, 2795.7796]

Hidroxide

O	0.000000	0.000000	0.107821
H	0.000000	0.000000	-0.862565

x3lyp:
Energy+ZPE (kcal/mol): -47635.003243903

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -47618.437633812

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -47639.26591254

Frequencies: [3749.3514]

Step 2 Product (3^-)

C	2.440972	0.297098	-0.258482
C	3.667551	0.946658	-0.018490
C	4.841599	0.215445	0.138198
C	4.812134	-1.182364	0.058082
C	3.602938	-1.839534	-0.180209
C	2.424822	-1.106747	-0.339758
C	1.208228	1.125842	-0.413910
C	-0.141239	0.505644	-0.658704
O	1.284268	2.361674	-0.312760
H	-0.081648	-0.513602	-1.045599
H	3.689714	2.029471	0.045808
H	5.779778	0.731113	0.323386
H	5.728148	-1.753958	0.180152
H	3.573929	-2.923587	-0.243468
H	1.499605	-1.639162	-0.524411
H	-0.649263	1.129953	-1.402567
C	-4.069179	-1.607917	-0.312100
C	-2.765393	-1.244080	0.034121
C	-2.433140	0.095339	0.290514
C	-3.445572	1.059898	0.192924
C	-4.754540	0.702722	-0.151236
C	-5.071208	-0.634423	-0.406344
H	-4.305231	-2.651221	-0.507968
H	-1.996728	-2.009177	0.112413
H	-3.207955	2.103283	0.392815
H	-5.525071	1.467395	-0.214820
H	-6.086703	-0.917067	-0.671691
C	-1.000953	0.493946	0.666500
O	-0.443172	-0.308713	1.654118
H	-1.049465	1.557717	0.978444

x3lyp:
Energy+ZPE (kcal/mol): -457738.73987048503

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457863.615416503

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -457872.343439184

Frequencies: [15.6941, 23.5257, 31.0917, 54.5047, 78.2223, 139.908, 171.0219, 218.4688, 224.3116, 268.7407, 347.3408, 398.6114, 412.33, 415.2185, 434.1133, 478.5108, 498.7498, 536.6241, 608.858, 629.7748, 631.15, 638.4544, 692.0695, 697.6173, 711.5878, 754.38, 778.0355, 784.8965, 859.3423, 861.2702, 878.6737, 880.2545, 930.5083, 958.1947,

988.3784, 994.2514, 999.9001, 1007.0891, 1013.6017, 1015.2779, 1020.8706, 1022.7976, 1048.9745, 1052.6965, 1094.8782, 1110.113, 1129.5097, 1175.0372, 1179.2414, 1192.7818, 1195.0503, 1204.1715, 1213.1374, 1264.3331, 1298.6928, 1316.9986, 1343.5729, 1350.3769, 1358.4298, 1367.2991, 1397.8453, 1482.4021, 1488.0712, 1499.6428, 1529.2865, 1538.0477, 1615.307, 1631.7523, 1640.3922, 1647.8138, 1657.3407, 2879.3217, 3075.5586, 3144.6937, 3175.6776, 3183.4779, 3192.3915, 3198.8716, 3199.9642, 3208.9599, 3210.8704, 3219.0188, 3229.1388, 3244.8975]

Deuterated Step 2 Product (3^-)

C	2.440972	0.297098	-0.258482
C	3.667551	0.946658	-0.018490
C	4.841599	0.215445	0.138198
C	4.812134	-1.182364	0.058082
C	3.602938	-1.839534	-0.180209
C	2.424822	-1.106747	-0.339758
C	1.208228	1.125842	-0.413910
C	-0.141239	0.505644	-0.658704
O	1.284268	2.361674	-0.312760
H(Iso=2)	-0.081648	-0.513602	-1.045599
H	3.689714	2.029471	0.045808
H	5.779778	0.731113	0.323386
H	5.728148	-1.753958	0.180152
H	3.573929	-2.923587	-0.243468
H	1.499605	-1.639162	-0.524411
H(Iso=2)	-0.649263	1.129953	-1.402567
C	-4.069179	-1.607917	-0.312100
C	-2.765393	-1.244080	0.034121
C	-2.433140	0.095339	0.290514
C	-3.445572	1.059898	0.192924
C	-4.754540	0.702722	-0.151236
C	-5.071208	-0.634423	-0.406344
H	-4.305231	-2.651221	-0.507968
H	-1.996728	-2.009177	0.112413
H	-3.207955	2.103283	0.392815
H	-5.525071	1.467395	-0.214820
H	-6.086703	-0.917067	-0.671691
C	-1.000953	0.493946	0.666500
O	-0.443172	-0.308713	1.654118
H	-1.049465	1.557717	0.978444

x3lyp:
Energy+ZPE (kcal/mol): -457742.97492872603

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457867.753210849

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -457876.50633389

Frequencies: [15.7035, 23.5059, 30.9015, 53.4853, 77.4511, 139.3842, 170.2478, 215.8646, 223.3064, 262.8181, 343.7984, 368.5305, 412.1619, 415.176, 428.8005, 451.4078, 482.2097, 525.1789, 581.6268, 617.4374, 629.7084, 632.0785, 689.3601, 694.0139, 711.5279, 743.5447, 744.3955, 777.0191, 802.4254, 859.0492, 861.1585, 867.3946, 874.6606, 916.3096, 951.2561, 956.8757, 988.4305, 999.1686, 1002.4452, 1007.066, 1013.6973, 1015.2731,

1021.3383, 1034.587, 1049.113, 1052.9453, 1095.4808, 1111.9222, 1138.3056, 1154.1262, 1175.1088, 1180.2591, 1192.9356, 1204.9758, 1210.3067, 1286.183, 1298.3608, 1338.4841, 1351.0834, 1358.4268, 1368.2108, 1395.8194, 1483.1642, 1487.9591, 1529.2689, 1533.322, 1613.1102, 1631.7295, 1638.947, 1647.7925, 1656.2337, 2239.6423, 2330.2876, 2879.5851, 3175.6776, 3183.4673, 3192.3841, 3198.8675, 3199.9568, 3208.9398, 3210.8698, 3218.9931, 3229.1368, 3244.2645]

Step 3 Product (3)

C	-2.863422	-0.828978	0.856788
C	-2.547003	0.244761	0.009216
C	-3.453595	0.598668	-0.998258
C	-4.651384	-0.105012	-1.162489
C	-4.958822	-1.170247	-0.312336
C	-4.061504	-1.529177	0.699951
H	-2.173238	-1.120306	1.645732
H	-3.220021	1.430422	-1.659145
H	-5.342698	0.182204	-1.950383
H	-5.889801	-1.717095	-0.435525
H	-4.293710	-2.356921	1.364873
C	1.288630	0.891959	-0.131338
C	2.569371	0.124207	-0.116658
C	2.596011	-1.281165	-0.084233
C	3.785809	0.830095	-0.146515
C	3.813631	-1.963337	-0.085399
H	1.673124	-1.850609	-0.066071
C	4.999993	0.147818	-0.140077
H	3.769722	1.914929	-0.170316
C	5.016289	-1.251675	-0.110782
H	3.822364	-3.049352	-0.065292
H	5.933162	0.703628	-0.157969
H	5.963149	-1.784575	-0.107567
O	1.298939	2.117934	-0.271565
C	-0.019955	0.132673	-0.001879
H	-0.134358	-0.476171	-0.909684
H	0.046969	-0.579760	0.829511
C	-1.252429	1.022920	0.175543
H	-1.229924	1.823749	-0.566128
O	-1.209372	1.713040	1.444222
H	-1.211001	1.051013	2.157487

x3lyp:
Energy+ZPE (kcal/mol): -458036.25130002

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -458178.22646628803

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -458173.613647629

Frequencies: [24.6002, 32.1865, 55.9792, 63.6115, 93.6393, 150.1169, 155.7795, 205.8016, 220.3549, 282.2089, 329.7647, 346.7338, 360.2439, 413.004, 418.9922, 426.8407, 463.2263, 521.2259, 564.2672, 595.4401, 617.0554, 629.6539, 633.8576, 675.6568, 695.9392, 715.5407, 769.6056, 771.1283, 794.1357, 864.363, 866.1065, 877.7775, 894.9135, 941.0663,

959.7027, 994.5472, 1003.0464, 1005.0368, 1013.0087, 1015.8083, 1016.1218, 1018.5787, 1024.8746, 1053.7495, 1056.698, 1090.0774, 1108.6236, 1114.4846, 1178.2586, 1179.5278, 1201.3912, 1204.1522, 1208.3775, 1229.6237, 1236.1195, 1295.1472, 1331.9161, 1349.5731, 1364.3412, 1367.606, 1373.024, 1418.7282, 1429.1103, 1454.0926, 1484.8916, 1492.805, 1534.7348, 1538.5232, 1627.1289, 1635.8758, 1646.789, 1655.8761, 1686.1529, 3055.1192, 3097.4704, 3126.9529, 3185.4216, 3187.5677, 3198.0898, 3201.2206, 3206.7723, 3210.1547, 3217.0328, 3219.3886, 3228.6055, 3236.3595, 3712.7828]

Deuterated Step 3 Product (3)

C	-2.863422	-0.828978	0.856788
C	-2.547003	0.244760	0.009216
C	-3.453595	0.598668	-0.998257
C	-4.651385	-0.105012	-1.162487
C	-4.958823	-1.170246	-0.312334
C	-4.061505	-1.529176	0.699952
H	-2.173237	-1.120306	1.645731
H	-3.220022	1.430422	-1.659145
H	-5.342699	0.182205	-1.950381
H	-5.889802	-1.717093	-0.435522
H	-4.293710	-2.356920	1.364875
C	1.288630	0.891959	-0.131339
C	2.569371	0.124207	-0.116658
C	2.596011	-1.281165	-0.084236
C	3.785810	0.830095	-0.146512
C	3.813631	-1.963337	-0.085402
H	1.673125	-1.850609	-0.066077
C	4.999993	0.147819	-0.140073
H	3.769722	1.914930	-0.170311
C	5.016290	-1.251674	-0.110781
H	3.822365	-3.049352	-0.065297
H	5.933162	0.703629	-0.157962
H	5.963150	-1.784574	-0.107566
O	1.298939	2.117933	-0.271566
C	-0.019955	0.132672	-0.001881
H(Iso=2)	-0.134357	-0.476171	-0.909686
H(Iso=2)	0.046969	-0.579762	0.829509
C	-1.252429	1.022920	0.175542
H	-1.229924	1.823749	-0.566129
O	-1.209371	1.713039	1.444221
H(Iso=2)	-1.211003	1.051012	2.157486

x3lyp:
Energy+ZPE (kcal/mol): -458042.518859912

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -458184.4187251

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -458179.859872215

Frequencies: [24.3854, 32.105, 55.6787, 62.5776, 86.9213, 148.4597, 152.9132, 203.8658, 218.4629, 248.7387, 271.7293, 318.6552, 352.8976, 407.4944, 415.7429, 418.7982, 454.8794, 485.7179, 548.695, 564.1249, 597.6825, 629.5929, 632.8005, 671.3233, 695.4573,

715.1441, 752.1109, 761.6495, 780.0849, 800.1788, 839.3202, 864.3107, 866.0948, 908.604, 932.1913, 940.9683, 960.0918, 973.36, 994.8404, 1003.1272, 1013.5404, 1015.8326, 1015.9788, 1024.2932, 1025.11, 1051.7773, 1055.5606, 1067.6747, 1081.0374, 1114.0755, 1126.5311, 1168.8358, 1178.3105, 1180.7475, 1204.2417, 1207.4578, 1231.2612, 1291.1839, 1323.7165, 1351.6509, 1364.5299, 1368.0159, 1377.6117, 1400.4847, 1484.58, 1492.6399, 1533.8935, 1538.2376, 1626.7232, 1635.773, 1646.392, 1655.849, 1683.6682, 2225.7147, 2293.0257, 2703.4925, 3125.8171, 3185.3866, 3187.5548, 3198.0856, 3201.2191, 3206.7696, 3210.1497, 3217.0324, 3219.3811, 3228.6039, 3236.2879]

Step 4 Product (5)

C	-2.176310	-0.349997	0.344883
C	-2.812844	0.505157	1.261386
C	-3.792404	1.407143	0.841521
C	-4.170611	1.458116	-0.505358
C	-3.557989	0.602185	-1.424264
C	-2.567350	-0.291434	-1.002260
C	-1.155242	-1.346008	0.842289
C	0.123246	-1.383819	0.331046
O	-1.581632	-2.146990	1.793655
H	-2.529840	0.466241	2.310301
H	-4.262087	2.069431	1.564496
H	-4.938051	2.154622	-0.832670
H	-3.851587	0.625474	-2.470735
H	-2.104960	-0.958772	-1.724877
H	0.797445	-2.136115	0.743382
C	4.439720	-0.275036	0.154478
C	3.196354	-0.770222	-0.244995
C	2.072789	0.070504	-0.297647
C	2.228226	1.418533	0.053229
C	3.470689	1.917038	0.458619
C	4.581998	1.071278	0.510342
H	5.298979	-0.940185	0.188208
H	3.098770	-1.817585	-0.517936
H	1.368324	2.083434	0.010411
H	3.569857	2.965877	0.726597
H	5.549799	1.455894	0.821114
C	0.705268	-0.461020	-0.689585
O	0.877365	-1.119512	-1.999461
H	0.040793	0.395142	-0.842882
H	0.083458	-1.665957	-2.131060

x3lyp:
Energy+ZPE (kcal/mol): -457734.765228479

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457869.451250203

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -457873.304155463

Frequencies: [25.901, 35.364, 39.0577, 60.93, 91.203, 147.7506, 182.4336, 210.5718, 224.7636, 274.5045, 302.5908, 359.1223, 366.7098, 413.0445, 415.3452, 418.978, 463.214, 545.3689, 573.2404, 614.9793, 630.185, 633.3604, 646.7632, 672.5417, 712.4765, 715.0037, 754.8601, 777.7459, 787.4818, 799.8807, 841.7014, 862.3397, 865.1218, 895.5887, 938.9013, 940.8967, 990.8568, 991.9791, 1008.6642, 1009.3312, 1014.3569, 1014.7382, 1048.517,

1051.7049, 1093.7883, 1102.9778, 1120.3217, 1157.4626, 1175.6768, 1177.1088, 1190.7937, 1199.7235, 1200.9495, 1228.9054, 1247.3567, 1324.2341, 1340.7214, 1343.5602, 1359.1446, 1361.8354, 1362.9372, 1413.9897, 1476.1271, 1491.5655, 1527.0741, 1536.0387, 1567.6675, 1625.6172, 1633.9384, 1649.619, 1653.6131, 3077.4832, 3138.734, 3185.6327, 3187.3706, 3191.3103, 3192.5344, 3199.6466, 3201.0714, 3206.4326, 3206.7658, 3214.8485, 3215.2279, 3720.0145]

Deuterated Step 4 Product (5)

C	-2.176310	-0.349997	0.344883
C	-2.812844	0.505157	1.261386
C	-3.792404	1.407143	0.841521
C	-4.170611	1.458116	-0.505358
C	-3.557989	0.602185	-1.424264
C	-2.567350	-0.291434	-1.002260
C	-1.155242	-1.346008	0.842289
C	0.123246	-1.383819	0.331046
O	-1.581632	-2.146990	1.793655
H	-2.529840	0.466241	2.310301
H	-4.262087	2.069431	1.564496
H	-4.938051	2.154622	-0.832670
H	-3.851587	0.625474	-2.470735
H	-2.104960	-0.958772	-1.724877
H(Iso=2)	0.797445	-2.136115	0.743382
C	4.439720	-0.275036	0.154478
C	3.196354	-0.770222	-0.244995
C	2.072789	0.070504	-0.297647
C	2.228226	1.418533	0.053229
C	3.470689	1.917038	0.458619
C	4.581998	1.071278	0.510342
H	5.298979	-0.940185	0.188208
H	3.098770	-1.817585	-0.517936
H	1.368324	2.083434	0.010411
H	3.569857	2.965877	0.726597
H	5.549799	1.455894	0.821114
C	0.705268	-0.461020	-0.689585
O	0.877365	-1.119512	-1.999461
H	0.040793	0.395142	-0.842882
H(Iso=2)	0.083458	-1.665957	-2.131060

x3lyp:
Energy+ZPE (kcal/mol): -457738.795718786

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457873.53947133804

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -457877.418731976

Frequencies: [25.868, 35.2117, 38.8079, 60.5945, 91.0246, 141.4878, 178.9934, 207.6765, 212.3953, 223.9107, 290.4288, 345.772, 357.8497, 404.0851, 415.2825, 418.4727, 441.1538, 524.2196, 564.4987, 589.8028, 600.6114, 631.8119, 632.6942, 639.1189, 712.381, 714.8041, 726.2647, 738.2725, 776.7339, 789.6947, 801.2616, 862.2288, 864.9128, 889.0379, 937.6024, 939.8779, 957.7075, 989.389, 990.9061, 993.6228, 1008.879, 1009.3749, 1014.6573,

1015.0681, 1048.9979, 1053.0455, 1100.4683, 1103.2171, 1116.5659, 1175.7143, 1177.1439, 1184.0106, 1199.716, 1200.5802, 1232.9765, 1289.0761, 1322.2546, 1333.5433, 1347.4965, 1360.2832, 1362.2208, 1397.0099, 1475.457, 1491.3269, 1523.0033, 1535.8227, 1554.0408, 1625.3513, 1633.9283, 1649.5622, 1653.5397, 2313.3304, 2707.8559, 3077.8308, 3185.6327, 3187.3732, 3191.3047, 3192.5438, 3199.637, 3201.0811, 3206.4503, 3206.7547, 3214.8518, 3215.2233]

Step 5 Product (4)

C	2.483423	-0.233699	-0.021463
C	3.657421	-0.948862	0.279578
C	4.892689	-0.306303	0.309891
C	4.977639	1.061671	0.025253
C	3.820149	1.781310	-0.282901
C	2.579218	1.142025	-0.298868
C	1.185939	-0.975856	-0.057276
C	-0.072639	-0.217042	0.008019
O	1.194025	-2.220076	-0.125911
H	3.589904	-2.009647	0.498152
H	5.789209	-0.868898	0.554839
H	5.941410	1.562966	0.044103
H	3.881187	2.841479	-0.511523
H	1.696665	1.720294	-0.549498
C	-5.015207	-0.564946	-0.082206
C	-3.719694	-1.079460	-0.136357
C	-2.597906	-0.234785	-0.014731
C	-2.814409	1.148298	0.163785
C	-4.107882	1.660194	0.216930
C	-5.213025	0.807130	0.094309
H	-5.866965	-1.232557	-0.177137
H	-3.564808	-2.146736	-0.273777
H	-1.971498	1.825618	0.260933
H	-4.258737	2.727332	0.354450
H	-6.220171	1.212463	0.136817
C	-1.270660	-0.840754	-0.080401
H	-0.013132	0.855659	0.146656
H	-1.265602	-1.920897	-0.218098

x3lyp:
Energy+ZPE (kcal/mol): -410102.619660562

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -410233.642284744

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -410226.311724606

Frequencies: [24.8492, 35.8343, 62.9029, 87.6457, 108.7608, 158.4735, 221.0695, 223.9678, 276.874, 310.8827, 413.6168, 415.2877, 419.2827, 451.9101, 497.8355, 534.2752, 576.3713, 629.1708, 631.0874, 679.0623, 688.7914, 698.1117, 712.58, 765.5693, 808.5725, 809.6245, 858.8652, 866.4037, 898.2396, 908.161, 948.5747, 961.9087, 996.3236, 1004.0368, 1013.4927, 1014.7942, 1016.0833, 1023.5987, 1028.9881, 1044.1104, 1053.3974, 1069.4058, 1110.7992, 1115.8241, 1179.6462, 1180.9663, 1202.2192, 1208.7724, 1238.3808, 1257.863, 1330.6754, 1340.7311, 1363.6746, 1366.5112, 1378.0145, 1394.4584, 1480.8386, 1488.9405, 1533.9434, 1539.0424, 1576.0633, 1624.9614, 1630.9149, 1648.6963, 1652.1166, 1687.6242,

3183.5469, 3197.1372, 3200.5112, 3202.1756, 3209.2871, 3210.4764, 3218.2676, 3219.0975, 3224.3803, 3228.1396, 3230.457, 3243.956]

Deuterated Step 5 Product (4)

C	2.483423	-0.233699	-0.021463
C	3.657421	-0.948862	0.279578
C	4.892689	-0.306303	0.309891
C	4.977639	1.061671	0.025253
C	3.820149	1.781310	-0.282901
C	2.579218	1.142025	-0.298868
C	1.185939	-0.975856	-0.057276
C	-0.072639	-0.217042	0.008019
O	1.194025	-2.220076	-0.125911
H	3.589904	-2.009647	0.498152
H	5.789209	-0.868898	0.554839
H	5.941410	1.562966	0.044103
H	3.881187	2.841479	-0.511523
H	1.696665	1.720294	-0.549498
C	-5.015207	-0.564946	-0.082206
C	-3.719694	-1.079460	-0.136357
C	-2.597906	-0.234785	-0.014731
C	-2.814409	1.148298	0.163785
C	-4.107882	1.660194	0.216930
C	-5.213025	0.807130	0.094309
H	-5.866965	-1.232557	-0.177137
H	-3.564808	-2.146736	-0.273777
H	-1.971498	1.825618	0.260933
H	-4.258737	2.727332	0.354450
H	-6.220171	1.212463	0.136817
C	-1.270660	-0.840754	-0.080401
H(Iso=2)	-0.013132	0.855659	0.146656
H	-1.265602	-1.920897	-0.218098

x3lyp:
Energy+ZPE (kcal/mol): -410104.70173542405

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -410235.67792394

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -410228.35301138303

Frequencies: [24.7356, 35.8127, 62.7248, 87.6347, 102.1486, 156.8874, 215.384, 223.4516, 274.3056, 309.9309, 413.2019, 415.0173, 417.8427, 448.4192, 493.8009, 520.4249, 574.4978, 629.0627, 630.6946, 664.5575, 680.5667, 697.9638, 702.2456, 745.7962, 783.2446, 806.218, 825.3982, 858.8116, 866.0343, 881.6632, 943.2052, 956.4202, 960.9673, 995.3726, 1003.5805, 1004.3321, 1014.4293, 1015.0207, 1018.2984, 1023.9255, 1049.7755, 1054.8657, 1098.5002, 1113.4587, 1140.7471, 1179.8885, 1181.4063, 1202.4879, 1211.6888, 1238.1026, 1288.3005, 1328.8496, 1349.6758, 1365.8891, 1368.4617, 1377.5497, 1480.7795, 1486.3355, 1533.1245, 1538.9863, 1575.4866, 1622.0376, 1630.8601, 1647.6981, 1652.083, 1669.1209, 2392.9656, 3183.7495, 3197.1415, 3200.5285, 3202.2447, 3209.3751, 3210.6077, 3218.6935, 3219.4729, 3225.3102, 3228.2615, 3233.2337]

Step 1 TS (1‡)

C	0.275958	0.322706	0.133960
C	1.354086	1.163846	-0.188941
C	2.647719	0.654128	-0.310881
C	2.883509	-0.711970	-0.126503
C	1.817507	-1.561349	0.186604
C	0.525925	-1.047972	0.321043
C	-1.106459	0.909330	0.262536
C	-2.133745	0.159675	0.926544
O	-1.328110	2.025351	-0.294080
H	-2.667915	-0.683609	0.006242
H	1.174776	2.224376	-0.335101
H	3.470885	1.321958	-0.550767
H	3.889176	-1.111421	-0.226743
H	1.990725	-2.625407	0.323634
H	-0.290801	-1.722462	0.556813
H	-2.986780	0.773444	1.228428
H	-1.801406	-0.518141	1.715334
O	-3.227455	-1.524112	-0.795252
H	-3.921136	-0.999015	-1.229345

x3lyp:
Energy+ZPE (kcal/mol): -288967.26071591

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -289034.09356195503

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -289041.582254361

Frequencies: [-1441.7715, 43.4195, 54.2338, 110.4409, 155.5004, 158.3006, 239.114, 378.7973, 414.4768, 418.5133, 474.9098, 503.448, 513.3227, 610.3036, 630.789, 680.9753, 704.6916, 733.4368, 769.4593, 788.8777, 864.4658, 935.6043, 961.3383, 997.629, 1014.7833, 1016.434, 1048.8224, 1052.1569, 1110.3575, 1126.4586, 1178.1965, 1200.4239, 1293.4936, 1339.9294, 1346.6326, 1362.555, 1474.6123, 1481.2038, 1531.0104, 1542.5576, 1563.7577, 1633.9059, 1650.1312, 3098.403, 3168.6272, 3194.3895, 3202.2948, 3213.6878, 3222.4459, 3226.3858, 3739.8122]

Deuterated Step 1 TS (1‡)

C	0.275958	0.322706	0.133960
C	1.354086	1.163846	-0.188941
C	2.647719	0.654128	-0.310881
C	2.883509	-0.711970	-0.126503
C	1.817507	-1.561349	0.186604
C	0.525925	-1.047972	0.321043
C	-1.106459	0.909330	0.262536
C	-2.133745	0.159675	0.926544
O	-1.328110	2.025351	-0.294080
H(Iso=2)	-2.667915	-0.683609	0.006242
H	1.174776	2.224376	-0.335101
H	3.470885	1.321958	-0.550767
H	3.889176	-1.111421	-0.226743
H	1.990725	-2.625407	0.323634

H	-0.290801	-1.722462	0.556813
H(Iso=2)	-2.986780	0.773444	1.228428
H(Iso=2)	-1.801406	-0.518141	1.715334
O	-3.227455	-1.524112	-0.795252
H	-3.921136	-0.999015	-1.229345

x3lyp:
Energy+ZPE (kcal/mol): -288972.350441409

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -289039.09104363096

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -289046.578481019

Frequencies: [-1061.2303, 43.257, 53.8771, 107.9747, 153.9108, 157.053, 232.3164, 357.4255, 381.1495, 414.2585, 420.3321, 462.1084, 481.0954, 571.1846, 622.4938, 631.1814, 652.486, 700.4127, 730.0941, 755.2077, 850.7283, 864.3434, 870.1089, 945.932, 958.1793, 997.6091, 1014.634, 1016.3795, 1030.1285, 1054.308, 1108.5562, 1153.194, 1168.3181, 1178.7371, 1200.508, 1328.7035, 1351.0704, 1362.6227, 1474.3869, 1528.6604, 1540.9012, 1632.986, 1649.9626, 2252.9211, 2354.8485, 3194.3814, 3202.27, 3213.6628, 3222.4158, 3226.24, 3739.7713]

Step 2 TS (2‡)

C	2.357791	0.381747	-0.306563
C	3.612921	0.905213	0.053984
C	4.725596	0.076184	0.200415
C	4.606763	-1.302415	-0.004203
C	3.365642	-1.839566	-0.357975
C	2.254425	-1.007161	-0.510381
C	1.187575	1.317332	-0.454386
C	-0.056608	0.830846	-0.892285
O	1.351849	2.539508	-0.092897
H	-0.138175	-0.124816	-1.398174
H	3.710231	1.973455	0.216957
H	5.685743	0.505612	0.474744
H	5.471631	-1.950477	0.110006
H	3.259751	-2.909525	-0.516962
H	1.305301	-1.452152	-0.786879
H	-0.802007	1.573708	-1.161099
C	-4.057752	-1.543512	-0.398537
C	-2.771748	-1.327173	0.100133
C	-2.354874	-0.034486	0.452667
C	-3.252344	1.034589	0.305777
C	-4.540612	0.818958	-0.186987
C	-4.946613	-0.471939	-0.543869
H	-4.369095	-2.548470	-0.671861
H	-2.085060	-2.160711	0.218813
H	-2.936032	2.038359	0.581899
H	-5.227838	1.654628	-0.290503
H	-5.948532	-0.642020	-0.928878
C	-0.995646	0.212184	1.029619
O	-0.337998	-0.727833	1.573576
H	-0.843827	1.244196	1.382051

x3lyp:
Energy+ZPE (kcal/mol): -457729.455247321

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457857.125090916

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -457860.18043223704

Frequencies: [-281.6387, 20.472, 33.4638, 42.9574, 74.037, 81.7469, 103.5578, 171.0595, 208.3369, 229.3209, 251.3964, 359.5178, 402.7458, 416.7102, 417.5894, 434.5633, 461.97, 488.361, 528.5468, 605.2636, 629.7764, 631.4448, 647.399, 687.099, 704.212, 706.8244, 749.825, 768.2663, 786.1938, 797.6199, 817.2047, 839.877, 862.7655, 863.4343, 937.6682, 948.3581, 994.5948, 996.6928, 1012.1016, 1012.6503, 1013.5343, 1013.9814, 1033.9258, 1043.122, 1046.7782, 1050.8771, 1100.8377, 1108.1381, 1133.2913, 1175.5808, 1175.9046, 1187.1141, 1201.469, 1213.1728, 1328.4974, 1335.3366, 1339.8706, 1359.7147, 1361.5908, 1369.7731, 1428.842, 1467.7526, 1482.1796, 1510.5635, 1528.225, 1530.2352, 1554.1721, 1629.9957, 1635.2799, 1648.0273, 1648.8324, 3009.3635, 3169.6439, 3185.6357, 3192.4314, 3193.3128, 3200.3025, 3201.9834, 3209.947, 3213.2414, 3217.1604, 3225.2569, 3232.4357, 3258.9343]

Deuterated Step 2 TS (2‡)

C	2.357791	0.381747	-0.306563
C	3.612921	0.905213	0.053984
C	4.725596	0.076184	0.200415
C	4.606763	-1.302415	-0.004203
C	3.365642	-1.839566	-0.357975
C	2.254425	-1.007161	-0.510381
C	1.187575	1.317332	-0.454386
C	-0.056608	0.830846	-0.892285
O	1.351849	2.539508	-0.092897
H(Iso=2)	-0.138175	-0.124816	-1.398174
H	3.710231	1.973455	0.216957
H	5.685743	0.505612	0.474744
H	5.471631	-1.950477	0.110006
H	3.259751	-2.909525	-0.516962
H	1.305301	-1.452152	-0.786879
H(Iso=2)	-0.802007	1.573708	-1.161099
C	-4.057752	-1.543512	-0.398537
C	-2.771748	-1.327173	0.100133
C	-2.354874	-0.034486	0.452667
C	-3.252344	1.034589	0.305777
C	-4.540612	0.818958	-0.186987
C	-4.946613	-0.471939	-0.543869
H	-4.369095	-2.548470	-0.671861
H	-2.085060	-2.160711	0.218813
H	-2.936032	2.038359	0.581899
H	-5.227838	1.654628	-0.290503
H	-5.948532	-0.642020	-0.928878
C	-0.995646	0.212184	1.029619
O	-0.337998	-0.727833	1.573576
H	-0.843827	1.244196	1.382051

x3lyp:
Energy+ZPE (kcal/mol): -457733.49515026296

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457861.057689819

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -457864.138759009

Frequencies: [-280.4674, 20.3991, 33.3893, 42.9352, 73.1975, 81.3351, 102.4866, 170.0416, 207.7091, 229.0343, 245.1286, 350.8324, 374.5736, 416.1634, 417.374, 422.5015, 454.5929, 465.2525, 517.1476, 557.7493, 578.302, 611.5086, 629.8095, 631.4326, 665.1998, 698.5662, 704.5607, 711.7909, 733.1216, 771.7145, 809.697, 835.2662, 862.2177, 863.3733, 879.5799, 937.4974, 948.2958, 994.5549, 996.6706, 1008.4995, 1012.1501, 1013.4635, 1013.9032, 1015.8704, 1041.703, 1046.7816, 1053.863, 1100.8416, 1106.5377, 1170.3682, 1175.9024, 1177.8875, 1187.1103, 1201.3947, 1213.1646, 1328.9356, 1335.3073, 1351.8567, 1359.7315, 1362.8033, 1367.2136, 1435.3192, 1471.5765, 1497.4038, 1527.1283, 1530.1765, 1538.6945, 1629.6716, 1635.2679, 1648.0187, 1648.7695, 2305.3741, 2426.769, 3009.3647, 3185.6307, 3192.4251, 3193.3115, 3200.3023, 3201.9826, 3209.9475, 3213.2466, 3217.1603, 3225.2738, 3233.0547]

Step 3 TS ($3^{\ddagger}$)

C	2.968682	1.094720	0.243793
C	2.517804	-0.231738	0.223176
C	3.385123	-1.225307	-0.256512
C	4.667498	-0.904555	-0.709375
C	5.106700	0.423714	-0.686618
C	4.252327	1.420942	-0.207267
H	2.316390	1.876952	0.619494
H	3.053106	-2.261834	-0.270406
H	5.325254	-1.690578	-1.071990
H	6.105158	0.676944	-1.033400
H	4.584603	2.455835	-0.181354
C	-1.182125	-1.277442	-0.131637
C	-2.451945	-0.505315	-0.267071
C	-3.597058	-0.965193	0.411070
C	-2.552266	0.649658	-1.063214
C	-4.805978	-0.282740	0.305626
H	-3.526320	-1.853595	1.030105
C	-3.769423	1.324158	-1.179603
H	-1.693372	1.020768	-1.610855
C	-4.895672	0.863801	-0.493120
H	-5.678573	-0.641306	0.844310
H	-3.835144	2.209481	-1.805483
H	-5.839756	1.394796	-0.578518
O	-1.208783	-2.428281	0.324698
C	0.154378	-0.683520	-0.529267
H	0.591322	-1.349974	-1.282904
H	0.063073	0.310813	-0.968019
C	1.115081	-0.614703	0.695849
H	1.180839	-1.636928	1.095138
O	0.608678	0.218571	1.713021

O	-0.291309	2.395457	1.088800
H	-1.173567	2.231013	0.718629
H	0.179533	1.252756	1.348122

x3lyp:
Energy+ZPE (kcal/mol): -505678.704330771

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -505814.952849905

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -505822.36059364997

Frequencies: [-960.3315, 18.2439, 25.0576, 26.8644, 50.9926, 80.7095, 87.5863, 114.5959, 153.8314, 166.2199, 187.9745, 206.3209, 232.5193, 253.9414, 354.3985, 369.619, 411.8891, 415.9904, 427.2168, 471.6807, 504.8503, 543.285, 590.1372, 592.6019, 610.7729, 629.7418, 633.0658, 639.3278, 687.2786, 696.9913, 712.7533, 758.9712, 773.9321, 783.5174, 860.8319, 864.0739, 887.7688, 906.769, 932.6635, 959.3777, 992.1266, 999.4643, 1006.4415, 1010.6482, 1014.4923, 1015.2314, 1019.7613, 1044.2122, 1051.8089, 1058.5305, 1100.7285, 1112.0734, 1175.2806, 1178.9467, 1186.4335, 1196.783, 1199.8718, 1202.1259, 1250.2908, 1294.1155, 1307.2739, 1336.2567, 1346.4934, 1360.1939, 1362.8796, 1373.1109, 1388.5003, 1419.8306, 1478.1231, 1484.7902, 1489.6148, 1529.7838, 1532.3326, 1533.3222, 1622.4826, 1633.7431, 1642.1612, 1651.6339, 1666.2048, 3017.2481, 3073.9122, 3157.5318, 3178.8543, 3190.1258, 3198.6036, 3200.9627, 3210.0033, 3210.668, 3219.1249, 3219.3711, 3228.6986, 3237.6687, 3764.9805]

Deuterated Step 3 TS (3‡)

C	2.968382	1.094850	0.243707
C	2.517752	-0.231697	0.223252
C	3.385310	-1.225185	-0.256166
C	4.667685	-0.904270	-0.708920
C	5.106638	0.424082	-0.686325
C	4.252024	1.421232	-0.207238
H	2.315902	1.877026	0.619203
H	3.053485	-2.261774	-0.269931
H	5.325630	-1.690231	-1.071328
H	6.105094	0.677440	-1.033022
H	4.584110	2.456190	-0.181449
C	-1.182035	-1.277640	-0.132072
C	-2.451807	-0.505392	-0.267199
C	-3.596722	-0.964935	0.411492
C	-2.552271	0.649337	-1.063674
C	-4.805588	-0.282338	0.306306
H	-3.525869	-1.853160	1.030770
C	-3.769383	1.323958	-1.179826
H	-1.693534	1.020093	-1.611802
C	-4.895427	0.863972	-0.492754
H	-5.678026	-0.640614	0.845435
H	-3.835231	2.209082	-1.805975
H	-5.839467	1.395076	-0.577944
O	-1.208734	-2.428601	0.323945
C	0.154464	-0.683617	-0.529541
H(Iso=2)	0.591569	-1.349990	-1.283153

H(Iso=2)	0.063127	0.310752	-0.968207
C	1.115005	-0.614824	0.695716
H	1.180793	-1.637084	1.094911
O	0.608397	0.218305	1.712904
O	-0.291802	2.395163	1.088863
H(Iso=2)	-1.173821	2.230602	0.718179
H(Iso=2)	0.179174	1.252460	1.348073

x3lyp:
Energy+ZPE (kcal/mol): -505685.900603983

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -505822.20434390905

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -505829.553101808

Frequencies: [-698.0, 18.1053, 25.0366, 26.5385, 50.1406, 79.9059, 84.6616, 110.627, 132.7105, 154.7685, 163.9889, 202.6008, 226.7329, 247.8099, 331.0834, 356.8957, 411.3955, 415.9977, 421.1321, 431.2976, 452.1019, 493.3809, 534.9119, 567.9643, 591.4901, 616.8214, 629.6489, 632.7817, 684.5517, 694.1699, 712.6051, 749.4504, 755.356, 770.8585, 808.6017, 859.9712, 863.1494, 865.546, 891.7665, 920.8452, 956.4572, 958.6981, 991.4787, 992.5388, 999.5326, 1008.2799, 1014.3905, 1015.2673, 1019.548, 1020.2903, 1050.8585, 1052.6442, 1080.1671, 1097.5456, 1112.6081, 1114.8541, 1138.6401, 1175.3439, 1180.1396, 1197.1275, 1198.5135, 1201.7316, 1280.6664, 1293.1398, 1308.9707, 1346.1298, 1349.346, 1361.0994, 1366.4926, 1419.4471, 1482.8251, 1489.4744, 1531.2876, 1533.0307, 1621.8411, 1633.6629, 1641.1636, 1651.6116, 1664.0439, 2240.3459, 2337.1259, 2739.9221, 3017.5223, 3178.8543, 3190.1259, 3198.6051, 3200.9546, 3209.977, 3210.6672, 3219.1205, 3219.3256, 3228.6914, 3237.1016]

Step 4 TS (4‡)

C	-3.037995	-0.012144	0.917335
C	-2.451311	0.038471	-0.357139
C	-2.965440	-0.788787	-1.364390
C	-4.035562	-1.653307	-1.108405
C	-4.611401	-1.696440	0.164016
C	-4.108962	-0.870416	1.176425
H	-2.656912	0.626397	1.710590
H	-2.525488	-0.754797	-2.358960
H	-4.421453	-2.285546	-1.904073
H	-5.445635	-2.363138	0.365805
H	-4.551980	-0.895806	2.168880
C	1.252615	0.716046	-0.649209
C	2.490379	-0.034676	-0.230534
C	2.578842	-0.718875	0.994399
C	3.601629	-0.049621	-1.090063
C	3.746313	-1.399024	1.346851
H	1.742823	-0.709400	1.686031
C	4.764879	-0.738593	-0.743791
H	3.544748	0.475533	-2.038241
C	4.842081	-1.414438	0.478102
H	3.800908	-1.914280	2.302067
H	5.610687	-0.747342	-1.426199
H	5.748696	-1.947518	0.751688

O	1.366403	1.592694	-1.550877
C	0.009086	0.451965	0.028879
H	-0.070829	-0.555917	0.437445
H	0.061078	1.220015	1.154262
C	-1.270845	0.951363	-0.647273
H	-1.131388	0.991584	-1.733327
O	-1.575231	2.322916	-0.269579
O	-0.117588	2.093370	2.075682
H	-0.705084	1.647093	2.709798
H	-1.214669	2.452121	0.641195

x3lyp:
Energy+ZPE (kcal/mol): -505664.900387789

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -505805.121666402

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -505809.699972066

Frequencies: [-1455.2657, 13.6311, 27.5255, 36.2788, 56.197, 66.8221, 103.6861, 130.662, 164.4137, 193.8737, 198.246, 217.098, 226.8561, 274.2972, 323.6665, 360.5565, 414.8933, 415.7921, 421.1674, 480.0561, 492.9801, 549.7162, 574.8113, 608.3989, 630.5012, 631.3466, 660.7333, 665.5721, 679.2863, 703.2843, 712.5164, 736.8143, 776.9364, 800.4759, 810.4185, 861.8628, 863.1531, 881.6173, 925.3918, 932.7889, 952.5458, 979.0565, 990.2177, 996.9585, 1009.3549, 1014.5583, 1014.9089, 1017.1315, 1041.4812, 1051.6322, 1053.5142, 1100.5001, 1103.2852, 1120.9868, 1175.5316, 1177.5438, 1197.0282, 1197.4866, 1219.9885, 1241.3019, 1258.698, 1302.8431, 1338.4762, 1354.249, 1360.7428, 1361.7235, 1407.3189, 1441.2682, 1478.1071, 1490.5825, 1496.528, 1528.6333, 1532.2271, 1534.9929, 1568.1808, 1633.1405, 1634.2617, 1649.8228, 1652.9439, 3061.9975, 3144.1634, 3183.0813, 3189.1315, 3194.5712, 3197.6714, 3202.6589, 3204.2842, 3213.4524, 3214.2531, 3221.9703, 3226.5535, 3379.0875, 3738.8127]

Deuterated Step 4 TS (4‡)

C	-3.037996	-0.012143	0.917335
C	-2.451311	0.038471	-0.357139
C	-2.965440	-0.788789	-1.364389
C	-4.035562	-1.653308	-1.108403
C	-4.611401	-1.696440	0.164018
C	-4.108963	-0.870414	1.176426
H	-2.656914	0.626400	1.710589
H	-2.525487	-0.754801	-2.358958
H	-4.421451	-2.285549	-1.904071
H	-5.445635	-2.363138	0.365806
H	-4.551982	-0.895803	2.168880
C	1.252615	0.716046	-0.649210
C	2.490379	-0.034676	-0.230534
C	2.578842	-0.718874	0.994399
C	3.601629	-0.049621	-1.090063
C	3.746313	-1.399023	1.346852
H	1.742823	-0.709399	1.686031
C	4.764879	-0.738593	-0.743790

H	3.544748	0.475532	-2.038242
C	4.842081	-1.414437	0.478103
H	3.800908	-1.914279	2.302068
H	5.610687	-0.747343	-1.426198
H	5.748696	-1.947517	0.751690
O	1.366403	1.592693	-1.550877
C	0.009085	0.451965	0.028878
H(Iso=2)	-0.070829	-0.555916	0.437445
H(Iso=2)	0.061078	1.220016	1.154261
C	-1.270845	0.951362	-0.647273
H	-1.131388	0.991583	-1.733328
O	-1.575231	2.322916	-0.269581
O	-0.117588	2.093371	2.075680
H	-0.705084	1.647095	2.709797
H(Iso=2)	-1.214669	2.452121	0.641193

x3lyp:
Energy+ZPE (kcal/mol): -505670.259314649

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -505810.53016647307

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -505815.043211201

Frequencies: [-1070.6561, 13.6721, 27.4647, 35.9893, 55.9042, 66.1248, 102.5694, 129.2071, 162.5379, 190.0866, 196.6934, 216.2812, 223.4011, 272.2676, 318.3146, 357.8016, 414.8335, 415.5085, 418.8411, 444.7336, 481.4951, 492.3537, 523.1842, 562.6715, 596.3989, 626.259, 630.7391, 635.2095, 675.7443, 694.7299, 704.1126, 712.3446, 752.5964, 775.5764, 796.9308, 824.9825, 861.7948, 863.1122, 881.5138, 908.5717, 927.1358, 935.5889, 956.84, 979.2179, 990.2214, 996.9626, 1009.3739, 1014.6302, 1014.9313, 1017.1578, 1034.5559, 1051.614, 1052.7834, 1093.7989, 1104.9216, 1126.4683, 1140.6954, 1174.6513, 1175.7824, 1180.1972, 1197.4885, 1198.1597, 1228.6461, 1300.2369, 1337.2689, 1347.5238, 1360.3397, 1360.6986, 1371.6502, 1405.3359, 1477.3191, 1490.3982, 1529.8724, 1533.8738, 1551.648, 1632.7992, 1633.8419, 1649.7226, 1652.8877, 2315.1285, 2463.7517, 3062.6014, 3183.0814, 3189.1324, 3194.5646, 3197.6714, 3202.6423, 3204.2842, 3213.4316, 3214.2547, 3221.9556, 3226.4151, 3738.7167]

Step 5 TS (5‡)

C	2.648774	1.205467	0.278735
C	2.469349	-0.141691	-0.087328
C	3.546633	-0.822103	-0.682827
C	4.762168	-0.177106	-0.918142
C	4.927311	1.161388	-0.549434
C	3.866171	1.847876	0.052787
H	1.838693	1.751161	0.753792
H	3.424014	-1.865360	-0.963945
H	5.579560	-0.719487	-1.385841
H	5.873508	1.665445	-0.726852
H	3.988497	2.886875	0.347289
C	-1.263324	-0.942239	-0.040896
C	-2.559989	-0.177530	-0.084217
C	-2.714140	1.082871	0.519457

C	-3.669559	-0.752266	-0.728109
C	-3.941694	1.747902	0.478073
H	-1.883685	1.541776	1.046350
C	-4.892292	-0.082419	-0.782400
H	-3.564854	-1.726464	-1.195387
C	-5.033605	1.170721	-0.176980
H	-4.045303	2.715457	0.961876
H	-5.735041	-0.538152	-1.295430
H	-5.986925	1.691086	-0.212656
O	-1.319827	-2.207409	-0.136773
C	-0.043682	-0.216162	0.078420
H	-0.088303	0.864456	0.149140
C	1.193423	-0.858336	0.111942
H	1.215085	-1.903407	-0.175049
O	1.568247	-1.541043	2.064847
H	1.624133	-0.654006	2.457634

x3lyp:
Energy+ZPE (kcal/mol): -457725.917351579

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457849.13564632804

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -457855.92090114503

Frequencies: [-302.1757, 31.1699, 33.1876, 56.4452, 69.6493, 80.7095, 109.7709, 146.1972, 178.0385, 204.1884, 223.7052, 253.1367, 301.1895, 356.7785, 408.5093, 415.8871, 417.3511, 472.4897, 520.8757, 544.9752, 576.022, 630.6775, 632.2087, 676.2955, 697.4045, 703.0307, 705.8475, 715.5837, 759.7711, 796.4892, 811.8875, 824.4506, 861.4189, 862.2517, 908.8459, 940.6808, 948.7705, 994.2174, 995.7206, 1012.451, 1013.9991, 1014.2975, 1015.7326, 1048.0032, 1052.1387, 1052.6931, 1095.5214, 1103.6663, 1112.0238, 1176.717, 1178.7469, 1196.8333, 1203.4872, 1224.2541, 1238.1241, 1289.088, 1327.9922, 1338.0325, 1360.8092, 1367.23, 1386.2762, 1457.8122, 1487.9534, 1501.6362, 1531.9828, 1534.7382, 1578.461, 1629.6664, 1632.5775, 1649.2329, 1651.8042, 3191.1348, 3194.2522, 3196.3767, 3201.9506, 3204.6523, 3211.2361, 3212.6839, 3216.9008, 3219.6836, 3220.4338, 3222.4548, 3229.9053, 3744.9973]

Deuterated Step 5 TS ($5^{‡}$)

C	2.648774	1.205467	0.278735
C	2.469349	-0.141691	-0.087328
C	3.546633	-0.822103	-0.682827
C	4.762168	-0.177106	-0.918142
C	4.927311	1.161388	-0.549434
C	3.866171	1.847876	0.052787
H	1.838693	1.751161	0.753792
H	3.424014	-1.865360	-0.963945
H	5.579560	-0.719487	-1.385841
H	5.873508	1.665445	-0.726852
H	3.988497	2.886875	0.347289
C	-1.263324	-0.942239	-0.040896
C	-2.559989	-0.177530	-0.084217
C	-2.714140	1.082871	0.519457

C	-3.669559	-0.752266	-0.728109
C	-3.941694	1.747902	0.478073
H	-1.883685	1.541776	1.046350
C	-4.892292	-0.082419	-0.782400
H	-3.564854	-1.726464	-1.195387
C	-5.033605	1.170721	-0.176980
H	-4.045303	2.715457	0.961876
H	-5.735041	-0.538152	-1.295430
H	-5.986925	1.691086	-0.212656
O	-1.319827	-2.207409	-0.136773
C	-0.043682	-0.216162	0.078420
H(Iso=2)	-0.088303	0.864456	0.149140
C	1.193423	-0.858336	0.111942
H	1.215085	-1.903407	-0.175049
O	1.568247	-1.541043	2.064847
H(Iso=2)	1.624133	-0.654006	2.457634

x3lyp:
Energy+ZPE (kcal/mol): -457729.779669474

M08HX (solvent=acetonitrile):
Energy+ZPE (kcal/mol): -457853.060087614

M08HX (solvent=water):
Energy+ZPE (kcal/mol): -457859.866050228

Frequencies: [-301.7794, 31.0189, 33.0858, 56.0462, 67.4545, 78.7277, 105.3918, 130.5637, 152.5746, 199.8192, 223.2394, 248.8262, 299.7184, 330.1565, 406.5598, 415.6606, 417.1637, 444.0171, 497.1074, 526.2415, 538.6667, 584.6771, 628.9552, 631.1651, 639.78, 676.6504, 701.512, 707.2456, 725.5233, 781.3063, 809.442, 814.6007, 861.1425, 862.175, 886.4596, 940.2424, 948.1362, 957.3289, 994.2783, 995.754, 1012.4369, 1013.9913, 1014.5205, 1015.7291, 1041.7815, 1049.2061, 1052.6164, 1100.2841, 1105.1052, 1142.7125, 1176.9105, 1178.826, 1196.6834, 1204.0779, 1223.6579, 1245.4225, 1323.2061, 1337.6779, 1360.5594, 1363.6725, 1369.596, 1454.446, 1480.2644, 1499.8369, 1530.227, 1531.7217, 1554.9796, 1629.6162, 1631.8923, 1649.2225, 1651.7106, 2378.9873, 2726.9835, 3191.1459, 3194.2866, 3196.4552, 3202.1104, 3204.8946, 3212.5298, 3212.8641, 3219.2064, 3220.1523, 3220.784, 3223.2444]