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

Reply to the 'Comment on "Topography of the Free Energy Landscape on the Claisen-Schmidt Condensation: Solvent and Temperature Effect in the Rate-Controlling Step"' by N. D. Coutinho, H. G. Machado, V. H. Carvalho-Silva and W. A. da Silva, Phys. Chem. Chem. Phys., 2021, 23, 6738

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Cartesian coordinate of all stationary points with explicit water molecules

Enolate (2^-) with 3 explicit water

C	0.999078	0.439267	-0.054591
C	1.220561	-0.893406	-0.444367
C	2.514273	-1.413601	-0.541644
C	3.620223	-0.613639	-0.238907
C	3.415740	0.710803	0.166164
C	2.122134	1.228343	0.259296
C	-0.409207	0.967034	0.023267
C	-0.659888	2.302058	-0.097315
O	-1.357953	0.050584	0.186002
H	0.129730	3.021552	-0.277871
H	0.365437	-1.520661	-0.671577
H	2.657202	-2.445150	-0.852436
H	4.265153	1.338980	0.420963
H	1.983799	2.250305	0.597887
H	-1.676207	2.679313	-0.036640
H	4.626472	-1.017171	-0.307931
O	-1.255747	-1.661729	2.252841
H	-2.082744	-1.493123	2.721502
H	-1.257598	-1.031022	1.479950
O	-2.569455	-1.235689	-1.909689
H	-3.433113	-0.860727	-1.679689
H	-1.985196	-0.836861	-1.219540
O	-3.985554	0.545320	0.122399
H	-4.191072	1.478333	-0.016546
H	-2.989669	0.487186	0.198085

B2LYP:
Energy+ZPE (kcal/mol): -384304.33031669864

B3LYP:
Energy+ZPE (kcal/mol): -385034.116409965

Frequencies: [44.81; 57.12; 71.74; 80.41; 90.37; 100.78; 113.57; 149.62; 208.05; 237.62; 286.49; 352.23; 366.83; 494.54; 555.55; 597.63; 600.82; 622.92; 692.23; 736.06; 762.24; 880.49; 904.99; 911.83; 986.67; 1016.74; 1055.56; 1087.23; 1094.17; 1142.48; 1234.6; 1236.66; 1277.94; 1344.04; 1422.5; 1442.61; 1448.59; 1454.02; 1503.66; 1580.97; 1626.86; 1691.29; 1720.18; 1888.99; 1921.6; 1947.45; 2034.01; 2120.72; 2188.35; 2297.57; 2339.2; 2361.21; 2366.14; 2379.19; 2444.16; 4491.36; 4549.76; 4568.47; 4579.23; 4598.58; 4608.78; 4613.25; 4625.06; 4676.44; 4896.45; 5470.53; 5558.06; 5560.22]

Hydroxide with 3 explicit water

O	0.005595	-0.040073	0.653187
H	0.006165	-0.051999	1.619758
O	2.142473	-1.223555	-0.261072
H	1.319964	-0.753045	0.111212
H	2.805161	-0.533427	-0.388201
O	-2.086044	-1.316992	-0.247088
H	-2.704254	-0.640497	-0.550184
H	-1.280716	-0.811764	0.115496
O	-0.161502	2.412753	-0.215149
H	-0.078637	1.461120	0.137555
H	0.728145	2.672546	-0.484671

B2LYP:
Energy+ZPE (kcal/mol): -191221.2931371083

B3LYP:
Energy+ZPE (kcal/mol): -191536.442674329

Frequencies: [50.17; 51.43; 93.18; 130.79; 146.83; 156.06; 385.66; 420.09; 427.15; 664.22; 679.25; 743.45; 783.65; 793.95; 1496.74; 1505.91; 1520.72; 2346.34; 2380.38; 2390.58; 3940.37; 3955.17; 4209.53; 5524.14; 5555.17; 5555.65; 5556.85/]

Step 2 Product (3^-) with 3 explicit water

C	2.491871	-0.169794	0.530404
C	3.462293	-1.187884	0.487456
C	4.643786	-1.014201	-0.230353
C	4.877070	0.185262	-0.915096
C	3.922034	1.205207	-0.878491
C	2.735227	1.029653	-0.162518
C	1.238804	-0.402799	1.323340
C	0.104253	0.594852	1.246662
O	1.133401	-1.416086	2.019185
H	0.486550	1.616709	1.329743
H	3.270857	-2.112298	1.021811
H	5.382797	-1.809477	-0.258452
H	5.798395	0.322701	-1.473627
H	4.099136	2.137487	-1.406162
H	2.008773	1.834486	-0.145397
H	-0.561501	0.407014	2.092874
C	-3.098243	-2.455643	0.405578
C	-2.490752	-1.208117	0.564942
C	-1.411294	-0.823911	-0.246901
C	-0.961496	-1.721361	-1.224700
C	-1.566379	-2.973616	-1.389648
C	-2.637335	-3.345636	-0.573106
H	-3.932656	-2.735329	1.043456
H	-2.860289	-0.520159	1.320006

H	-0.133353	-1.436828	-1.870154
H	-1.203801	-3.652149	-2.157232
H	-3.111786	-4.314918	-0.698588
C	-0.744044	0.542085	-0.076756
O	-1.661926	1.594977	-0.078615
H	-0.036362	0.651799	-0.917837
O	-0.437945	3.896028	-0.438851
H	-0.909379	3.015327	-0.276830
H	-0.629718	4.439041	0.336016
O	-3.201819	2.202018	1.973541
H	-2.612455	1.922312	1.204140
H	-4.105781	2.023113	1.685846
O	-3.184358	1.772562	-2.219936
H	-2.931709	2.608793	-2.630720
H	-2.591317	1.681797	-1.406355

B2LYP:
Energy+ZPE (kcal/mol): -600685.3336635352

B3LYP:
Energy+ZPE (kcal/mol): -601842.020708306

Frequencies: [25.42; 37.12; 46.7; 54.38; 60.11; 65.36; 71.5; 78.33; 89.05; 99.61; 117.79; 134.57; 138.49; 176.2; 203.49; 241.29; 249.82; 272.73; 315.71; 354.55; 421.85; 476.97; 523.96; 556.89; 596.69; 598.02; 641.44; 649.93; 712.17; 732.21; 754.42; 772.57; 794.35; 878.94; 903.26; 905.73; 925.64; 983.54; 1009.27; 1025.17; 1084.92; 1104.42; 1115.47; 1175.33; 1239.93; 1242.64; 1333.94; 1355.73; 1384.69; 1399.72; 1417.49; 1423.42; 1426.08; 1439.28; 1445.01; 1455.84; 1456.0; 1458.91; 1464.0; 1499.39; 1506.71; 1536.98; 1560.04; 1588.62; 1601.75; 1666.6; 1691.96; 1696.61; 1722.9; 1726.11; 1743.29; 1838.37; 1850.56; 1900.19; 1927.95; 1948.47; 1953.79; 1957.72; 2007.15; 2125.92; 2134.48; 2136.08; 2194.47; 2196.04; 2331.54; 2340.3; 2359.5; 2366.16; 2366.64; 2385.7; 2401.0; 2442.38; 4127.66; 4186.36; 4221.93; 4391.87; 4417.63; 4500.05; 4557.12; 4568.99; 4582.22; 4585.14; 4595.06; 4598.9; 4606.23; 4613.05; 4627.66; 4632.26; 5554.07; 5554.73; 5555.53]

Step 4 Product (5) with 3 explicit water

C	1.699818	-0.720190	-0.055152
C	2.362950	-0.951566	1.163931
C	3.109929	-2.113961	1.365562
C	3.225180	-3.063154	0.342653
C	2.585803	-2.837734	-0.879449
C	1.829274	-1.677080	-1.075213
C	0.926645	0.558009	-0.239447
C	-0.372852	0.586931	-0.669200
O	1.594643	1.660495	0.079647
H	2.282827	-0.214454	1.957403
H	3.603569	-2.279025	2.319377

H	3.811656	-3.964567	0.495841
H	2.678783	-3.561005	-1.684912
H	1.350519	-1.507804	-2.034883
H	-0.841028	1.566865	-0.754249
C	-4.842492	0.479579	-0.128197
C	-3.621455	0.346630	-0.795234
C	-2.609002	-0.476426	-0.278652
C	-2.852226	-1.169866	0.915659
C	-4.071881	-1.037940	1.587238
C	-5.072596	-0.210825	1.067393
H	-5.615914	1.120482	-0.543018
H	-3.452357	0.876164	-1.727795
H	-2.079951	-1.817332	1.324530
H	-4.241615	-1.585114	2.510532
H	-6.022572	-0.109089	1.584394
C	-1.253555	-0.590239	-0.961483
O	-1.491974	-0.744525	-2.396274
H	-0.774196	-1.508227	-0.604320
H	-0.767223	-0.285393	-2.843495
O	1.053070	3.902247	-1.340397
H	1.920723	4.283782	-1.523952
H	1.233116	3.071443	-0.823257
O	4.282088	1.797361	-0.069401
H	4.641971	0.946694	0.211991
H	3.293016	1.692816	-0.006022
O	0.980521	2.748072	2.481265
H	1.183837	2.350615	1.594203
H	0.186823	3.280952	2.346454

B2LYP:
Energy+ZPE (kcal/mol): -600678.3961034988

B3LYP:
Energy+ZPE (kcal/mol): -601835.790798954

Frequencies: [19.4; 31.42; 38.72; 45.56; 52.44; 55.63; 63.07; 69.95; 77.81; 81.2; 93.64; 124.08; 146.01; 158.08; 208.71; 230.3; 257.54; 268.15; 289.75; 327.05; 344.88; 378.71; 444.58; 524.1; 540.79; 596.35; 600.98; 601.46; 629.43; 663.6; 702.28; 710.05; 782.1; 827.54; 890.97; 904.22; 909.4; 934.51; 961.6; 1020.71; 1025.73; 1082.69; 1126.37; 1132.52; 1137.51; 1177.04; 1195.1; 1209.84; 1221.17; 1234.48; 1239.67; 1331.6; 1348.23; 1364.45; 1419.09; 1424.19; 1442.38; 1447.27; 1454.72; 1455.28; 1503.02; 1505.77; 1565.88; 1580.77; 1589.92; 1658.24; 1690.3; 1692.4; 1707.8; 1719.19; 1723.55; 1772.78; 1808.64; 1902.87; 1906.93; 1943.93; 1949.5; 1949.9; 1962.36; 2015.11; 2117.27; 2134.73; 2190.66; 2196.3; 2300.73; 2334.12; 2340.4; 2347.78; 2364.57; 2368.4; 2374.07; 2403.3; 4396.11; 4532.12; 4562.79; 4572.19; 4573.35; 4582.32; 4586.86; 4597.33; 4602.55; 4603.27; 4605.22; 4611.97; 4613.54; 4659.42; 4766.51; 5468.91; 5557.05; 5558.32; 5560.97]

Step 1 TS (1‡) with 3 explicit water

C	-1.789061	-0.198163	0.278918
C	-2.897323	-0.968001	-0.114867
C	-4.060965	-0.357909	-0.584273
C	-4.130617	1.036680	-0.681914
C	-3.031378	1.813704	-0.302690
C	-1.871728	1.201718	0.179898
C	-0.554143	-0.904760	0.780483
C	0.534289	-0.144386	1.379902
O	-0.469578	-2.141570	0.591606
H	1.391627	0.121051	0.433361
H	-2.830057	-2.048279	-0.043251
H	-4.911843	-0.967047	-0.875791
H	-5.034074	1.513685	-1.050886
H	-3.076079	2.896043	-0.381774
H	-1.028162	1.820020	0.466408
H	1.115947	-0.763928	2.067927
H	0.243528	0.798507	1.845004
O	2.379508	0.304763	-0.473646
H	1.949339	0.534517	-1.311179
O	3.275435	2.636613	0.611984
H	2.930204	1.803305	0.190308
H	3.418891	3.255779	-0.114768
O	5.048837	-0.055543	-0.915281
H	5.466466	0.670486	-0.434427
H	4.074463	0.064639	-0.761967
O	2.192809	-2.545145	-0.452078
H	2.367509	-1.579362	-0.510374
H	1.311722	-2.585651	-0.032004

B2LYP:
Energy+ZPE (kcal/mol): -432173.886275471

B3LYP:
Energy+ZPE (kcal/mol): -432986.422717263

Frequencies: [-901.6647; 26.04; 28.34; 39.64; 54.53; 71.36; 78.9; 106.42; 159.97; 179.23; 200.27; 229.97; 243.38; 334.46; 352.7; 372.8; 543.15; 575.68; 596.07; 619.6; 642.33; 700.96; 716.66; 778.15; 808.34; 817.9; 847.88; 904.82; 915.41; 934.91; 998.32; 1018.78; 1068.87; 1086.27; 1137.61; 1209.6; 1239.83; 1240.9; 1362.19; 1427.79; 1434.1; 1456.57; 1457.59; 1496.81; 1504.15; 1587.91; 1605.76; 1694.94; 1721.27; 1878.12; 1922.67; 1952.32; 2072.12; 2120.04; 2137.86; 2178.49; 2192.92; 2310.35; 2353.6; 2370.36; 2377.57; 2383.85; 2442.17; 4439.29; 4540.32; 4579.11; 4591.86; 4608.46; 4626.0; 4626.4; 4629.44; 4740.49; 5043.69; 5228.77; 5480.32; 5553.58; 5558.88]

Step 2 TS ($2^{‡}$) with 3 explicit water

C	2.618109	-0.159510	0.439853

C	3.671057	-1.090491	0.406407
C	4.840868	-0.828787	-0.308345
C	4.979319	0.373206	-1.011824
C	3.938961	1.307509	-0.991516
C	2.770541	1.044809	-0.271046
C	1.377568	-0.499642	1.238084
C	0.332211	0.473652	1.367171
O	1.279852	-1.659630	1.713609
H	0.579451	1.525753	1.274048
H	3.552785	-2.020639	0.951996
H	5.644230	-1.560257	-0.317638
H	5.888206	0.579589	-1.569828
H	4.035253	2.242168	-1.536705
H	1.978625	1.785629	-0.272240
H	-0.426734	0.244606	2.109882
C	-3.334776	-2.425485	0.378494
C	-2.772979	-1.148692	0.335253
C	-1.538283	-0.932544	-0.300690
C	-0.883023	-2.023591	-0.894833
C	-1.446966	-3.301333	-0.856341
C	-2.674194	-3.507550	-0.217565
H	-4.289593	-2.578806	0.873981
H	-3.287248	-0.307786	0.790145
H	0.069092	-1.867890	-1.395459
H	-0.930270	-4.133979	-1.325440
H	-3.114102	-4.500253	-0.186772
C	-0.944552	0.431312	-0.385456
O	-1.711713	1.475628	-0.269705
H	-0.101932	0.500208	-1.085803
O	-0.709372	3.983015	-0.156731
H	-1.003234	4.499982	-0.917687
H	-1.014776	3.052284	-0.323705
O	-2.646903	2.930036	1.915536
H	-2.125941	3.676375	1.578472
H	-2.433445	2.227938	1.263949
O	-3.850506	1.736401	-1.991971
H	-3.084057	1.641909	-1.377886
H	-4.430344	0.992410	-1.785107

B2LYP:
Energy+ZPE (kcal/mol): -600662.6581288332

B3LYP:
Energy+ZPE (kcal/mol): -601825.0672976531

Frequencies: [-309.9222; 22.42; 30.48; 40.51; 51.9; 53.92; 59.38; 70.25; 74.48; 92.59; 109.15; 116.33; 121.33; 206.18; 217.52; 229.27; 232.15; 241.3; 281.85; 352.69; 359.89; 395.11; 504.54; 547.78; 564.19; 578.87; 586.83; 596.75; 600.14; 631.4; 650.54; 684.25; 713.49; 770.34; 869.45; 904.23; 906.05; 922.68; 969.1; 995.84; 1012.77; 1020.47; 1051.5; 1065.0; 1099.48; 1107.96; 1160.87; 1224.03; 1235.05; 1240.58; 1279.39; 1291.49;

1340.93; 1363.17; 1423.11; 1431.85; 1444.62; 1452.15; 1453.44; 1455.74; 1482.51; 1501.76; 1502.64; 1518.96; 1578.95; 1586.99; 1612.15; 1691.25; 1692.43; 1710.71; 1722.17; 1747.22; 1859.82; 1907.58; 1916.7; 1922.82; 1951.1; 1953.45; 2071.43; 2117.08; 2133.05; 2151.55; 2191.1; 2193.09; 2273.42; 2338.07; 2340.3; 2343.49; 2361.79; 2362.53; 2363.9; 2431.02; 4357.95; 4532.19; 4569.92; 4575.3; 4578.15; 4587.45; 4590.93; 4605.14; 4605.75; 4613.83; 4623.31; 4626.31; 4664.24; 4703.28; 4919.51; 5104.63; 5436.54; 5556.65; 5560.42]

Step 3 TS (3‡) with 3 explicit water

C	-2.803603	0.049309	0.640011
C	-2.189040	-0.991696	-0.069587
C	-2.806664	-2.252258	-0.077035
C	-4.002822	-2.472389	0.611782
C	-4.605719	-1.427225	1.320687
C	-4.002222	-0.165878	1.329524
H	-2.348140	1.034125	0.642713
H	-2.350119	-3.068922	-0.632646
H	-4.466853	-3.454724	0.588739
H	-5.537809	-1.592917	1.853481
H	-4.465161	0.654385	1.871665
C	1.622280	-1.336383	-0.699948
C	2.891906	-0.735510	-0.176276
C	4.082669	-0.979679	-0.888433
C	2.947555	0.048553	0.990382
C	5.295836	-0.456454	-0.448993
H	4.036055	-1.585384	-1.786993
C	4.166734	0.573447	1.429108
H	2.052801	0.266869	1.561896
C	5.340697	0.323226	0.714289
H	6.205840	-0.654119	-1.007737
H	4.195915	1.179470	2.329652
H	6.285897	0.732342	1.059267
O	1.633410	-1.966546	-1.758512
C	0.320315	-1.227925	0.083113
H	0.119641	-2.233818	0.474766
H	0.392029	-0.557599	0.940060
C	-0.866989	-0.787888	-0.812446
H	-0.874035	-1.457507	-1.682959
O	-0.682454	0.527553	-1.286904
O	-0.045550	2.285268	0.282348
H	0.833456	2.600797	0.031810
H	-0.355517	1.302365	-0.512500
O	-2.529687	1.824919	-2.692971
H	-1.878671	1.255785	-2.185147
H	-3.397139	1.424888	-2.549964
O	-1.909259	3.963217	-0.829096
H	-2.239479	3.360631	-1.523126

H	-1.214534	3.422537	-0.370339
O	0.193853	1.521337	2.812058
H	0.070599	1.823201	1.860277
H	-0.692873	1.334126	3.144641

B2LYP:
Energy+ZPE (kcal/mol): -648564.4801586191

B3LYP:
Energy+ZPE (kcal/mol): -649802.672257795

Frequencies: [-261.1389; 23.11; 25.26; 33.66; 52.62; 59.35; 63.98; 73.9; 87.93; 98.46; 112.45; 136.19; 149.74; 215.56; 229.86; 254.85; 296.5; 311.48; 344.8; 359.08; 370.27; 406.31; 426.11; 531.79; 538.94; 594.18; 598.0; 599.99; 628.21; 666.05; 725.88; 741.79; 773.53; 798.36; 851.88; 868.79; 899.81; 901.07; 902.45; 909.17; 946.39; 983.84; 1004.27; 1028.29; 1089.36; 1112.12; 1119.65; 1200.58; 1235.22; 1242.37; 1246.66; 1275.45; 1303.85; 1306.21; 1340.05; 1343.96; 1388.94; 1425.1; 1436.77; 1445.42; 1447.93; 1454.29; 1455.52; 1464.92; 1502.05; 1508.83; 1523.42; 1564.94; 1592.93; 1607.89; 1691.99; 1697.87; 1716.38; 1722.55; 1733.74; 1762.38; 1799.84; 1855.63; 1914.41; 1926.89; 1952.11; 1957.35; 1985.01; 2013.32; 2073.36; 2109.24; 2128.49; 2132.78; 2196.83; 2197.73; 2331.73; 2335.5; 2341.57; 2358.46; 2367.9; 2395.3; 2413.27; 2448.71; 2461.63; 4350.64; 4364.27; 4384.37; 4473.17; 4523.08; 4554.4; 4572.68; 4584.37; 4585.66; 4598.21; 4604.71; 4613.17; 4620.29; 4630.57; 4634.5; 4765.42; 5233.0; 5517.72; 5554.44; 5556.6]

Step 4 TS (4‡) with 3 explicit water

C	-3.544141	-0.154841	0.532770
C	-2.620262	-0.696420	-0.370796
C	-2.826918	-2.006751	-0.832175
C	-3.920295	-2.759689	-0.397005
C	-4.833328	-2.210989	0.511343
C	-4.640861	-0.905554	0.972569
H	-3.414102	0.863087	0.886692
H	-2.124941	-2.439759	-1.541621
H	-4.063469	-3.769887	-0.770961
H	-5.686667	-2.792164	0.849115
H	-5.346350	-0.466794	1.673145
C	1.097505	-0.352383	-0.798742
C	2.290828	-1.070528	-0.209828
C	2.365844	-1.437110	1.145006
C	3.371530	-1.382986	-1.051473
C	3.491954	-2.097650	1.643059
H	1.553553	-1.193432	1.821191
C	4.492522	-2.052744	-0.558657
H	3.315681	-1.093770	-2.095770
C	4.557106	-2.411354	0.792580
H	3.538185	-2.364671	2.695004
H	5.315698	-2.293427	-1.225558

H	5.430477	-2.928432	1.179722
O	1.227199	0.201085	-1.910184
C	-0.143068	-0.295465	-0.031198
H	-0.290707	-1.168575	0.607193
H	-0.010283	0.722039	0.827794
C	-1.393752	0.076255	-0.842069
H	-1.225138	-0.163528	-1.898334
O	-1.622225	1.502432	-0.833482
O	-0.070320	1.820586	1.522213
H	-0.308575	1.578318	2.428806
H	-1.362186	1.818867	0.052830
O	2.427051	2.807703	0.710632
H	2.074404	3.080969	-0.156349
H	1.635765	2.412424	1.142407
O	0.625452	3.528580	-1.526718
H	0.194715	2.662491	-1.634740
H	0.105168	3.960944	-0.816301
O	-0.722904	4.346578	0.835000
H	-0.478782	3.460148	1.222514
H	-0.234471	5.008688	1.341226

B2LYP:
Energy+ZPE (kcal/mol): -648545.3759608688

B3LYP:
Energy+ZPE (kcal/mol): -649784.993446738

Frequencies: [-1140.4278; 26.79; 41.84; 50.55; 54.41; 72.8; 86.09; 121.48; 125.9; 138.74; 165.82; 198.54; 200.19; 210.24; 268.25; 273.22; 292.59; 306.37; 330.21; 351.61; 381.16; 407.19; 467.57; 501.88; 559.32; 594.15; 595.49; 597.15; 612.22; 678.89; 694.18; 716.18; 745.99; 763.49; 801.5; 825.06; 851.67; 885.03; 905.24; 906.6; 937.08; 970.72; 982.29; 1008.57; 1016.33; 1022.6; 1036.26; 1084.71; 1105.87; 1130.63; 1147.38; 1234.72; 1240.15; 1267.6; 1327.83; 1351.86; 1372.88; 1398.55; 1418.45; 1425.64; 1431.62; 1442.35; 1454.02; 1454.72; 1456.12; 1499.08; 1509.54; 1515.97; 1562.66; 1586.17; 1592.82; 1692.33; 1692.95; 1718.87; 1722.63; 1736.26; 1765.1; 1800.68; 1851.64; 1914.71; 1926.0; 1950.42; 1953.82; 1989.82; 2053.33; 2103.53; 2123.73; 2129.71; 2190.79; 2197.48; 2240.83; 2319.81; 2339.09; 2356.02; 2361.2; 2368.24; 2378.2; 2411.06; 2446.22; 4387.72; 4483.17; 4557.76; 4572.17; 4575.98; 4585.16; 4588.31; 4601.8; 4603.13; 4605.63; 4611.7; 4620.82; 4624.81; 5008.47; 5106.47; 5203.25; 5296.71; 5384.98; 5498.94; 5555.59]

Step 5 TS (5‡) with 3 explicit water

C	-2.645177	-1.443984	0.917134
C	-2.447441	-0.761026	-0.298353
C	-3.519838	-0.694681	-1.207669
C	-4.746447	-1.297191	-0.920041

C	-4.927756	-1.972399	0.290838
C	-3.871684	-2.040288	1.208524
H	-1.842753	-1.496966	1.646141
H	-3.385934	-0.166439	-2.148066
H	-5.558765	-1.237374	-1.638639
H	-5.881518	-2.438455	0.520349
H	-4.006694	-2.556813	2.154549
C	1.309955	-0.139866	-0.770823
C	2.575643	-0.808528	-0.303769
C	2.590735	-2.084245	0.287656
C	3.796973	-0.137624	-0.490901
C	3.795902	-2.671083	0.681402
H	1.666991	-2.637000	0.421149
C	4.999390	-0.716924	-0.085162
H	3.785996	0.844219	-0.951957
C	5.002654	-1.987721	0.501514
H	3.791880	-3.662339	1.125241
H	5.932985	-0.179955	-0.226080
H	5.938362	-2.442585	0.813508
O	1.407713	0.747419	-1.656168
C	0.056714	-0.551814	-0.183299
H	0.097965	-1.223498	0.665667
C	-1.163236	-0.141633	-0.669761
H	-1.168029	0.412747	-1.600193
O	-1.721947	1.851108	0.173364
H	-2.687752	1.892171	0.147641
O	-0.084694	3.099361	-1.447900
H	0.439813	2.273145	-1.520925
H	-0.847467	2.763399	-0.881243
O	0.963672	4.414956	0.827103
H	0.690098	4.042521	-0.040730
H	0.465279	3.863560	1.468514
O	-0.677223	2.686613	2.354824
H	-0.233025	1.942318	2.780809
H	-1.135926	2.305729	1.510746

B2LYP:
Energy+ZPE (kcal/mol): -600665.7887448787

B3LYP:
Energy+ZPE (kcal/mol): -601832.695924566

Frequencies: [-101.5863; 16.94; 26.58; 40.7; 54.39; 59.96; 70.71; 84.47; 94.75; 135.5; 176.39; 213.09; 242.32; 250.58; 272.64; 319.1; 322.09; 360.44; 388.04; 395.47; 426.82; 457.86; 516.83; 580.47; 596.35; 596.55; 618.52; 656.58; 737.34; 763.11; 788.66; 807.09; 832.12; 859.08; 881.48; 905.11; 908.71; 968.88; 986.45; 999.13; 1007.46; 1021.73; 1028.81; 1095.84; 1148.92; 1156.09; 1165.36; 1213.01; 1231.27; 1239.55; 1306.18; 1344.05; 1366.54; 1422.14; 1432.4; 1446.03; 1451.05; 1454.82; 1456.23; 1456.56; 1483.71; 1503.02; 1508.19; 1558.57; 1584.73; 1595.57; 1644.16; 1695.37; 1696.19; 1722.3; 1728.3; 1762.59; 1783.61; 1873.0; 1907.19; 1927.7; 1952.76; 1959.65; 1983.64;

2116.7; 2130.77; 2188.68; 2197.87; 2218.56; 2315.07; 2334.89; 2355.04; 2364.86; 2366.22; 2368.31; 2445.91; 2472.61; 3618.88; 4355.33; 4574.51; 4580.45; 4582.67; 4592.64; 4595.24; 4606.39; 4608.24; 4616.02; 4619.26; 4628.03; 4631.31; 4640.27; 5016.41; 5081.93; 5116.24; 5513.88; 5547.13]