

Supporting Information for:

Spectroscopic and Computational Studies of Aqueous

Ethylene Glycol Solution Surfaces

Elizabeth Hommel, John K. Merle, Gang Ma, Christopher M. Hadad*, Heather C. Allen*

Department of Chemistry, 100 West 18th Avenue, The Ohio State University,
Columbus, Ohio 43210

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Correspondence info: CMH: hadad.1@osu.edu, Fax: (614) 292-1685

HCA: allen@chemistry.ohio-state.edu, Fax: (614) 292-1685

- S.1.** Cartesian coordinates (Angstrom) and vibrational frequencies (cm^{-1}) for all structures and complexes.
- S.2.** Energies, enthalpy, free energy corrections at 298 K, and moments of inertia for all structures and complexes.
- S.3.** Structural degeneracies, ΔH_0 , ΔG_{298} and 298 K Boltzmann weightings.
- S.4.** Boltzmann weightings based on SCF, H(0 K), and G(298 K) energies.

S.1.

Gas Phase Info.

g-G+g-

MP2 = -229.6180514

Cartesian Coordinates

O	0.000000	1.438264	-0.555260
C	0.352459	0.670546	0.601336
C	-0.352459	-0.670546	0.601336
O	0.000000	-1.438264	-0.555260
H	-0.565919	-1.148829	-1.281654
H	0.565919	1.148829	-1.281654
H	-1.433758	-0.519972	0.649163
H	1.433758	0.519972	0.649163
H	0.042411	1.257381	1.466509
H	-0.042411	-1.257381	1.466509

Vibrational Frequencies

-92.0780	162.2362	322.1637
428.0749	536.9095	888.7443
898.2750	1056.3377	1066.9833
1133.2007	1196.3725	1271.1184
1389.9577	1392.9752	1425.5693
1450.5888	1535.7791	1540.5176
3120.8930	3121.6195	3193.8621
3202.3794	3888.2970	3889.9954

g+G+g-

MP2 = -229.619048

Cartesian Coordinates

C	0.722556	0.575586	0.289213
H	0.668009	0.591820	1.385147
H	1.288843	1.448294	-0.036119
C	-0.675568	0.601930	-0.293774
H	-0.625697	0.599539	-1.380840
H	-1.219717	1.491748	0.035748
O	-1.383590	-0.599262	0.053112
H	-1.668159	-0.532909	0.974277
O	1.438970	-0.568763	-0.161872
H	0.831755	-1.319385	-0.080777

Vibrational Frequencies

175.4624	295.8920	336.5899
477.9587	545.0663	888.6924
906.6381	1068.5888	1078.3462
1128.5322	1210.0385	1253.0361
1384.4207	1386.9280	1425.4927
1459.8613	1541.7115	1552.8601
3075.6688	3117.1079	3189.2507
3218.5281	3835.3856	3870.9270

g+G+g+

MP2 = -229.6143213

Cartesian Coordinates

O	-0.559888	1.330523	-0.596157
C	0.000000	0.758913	0.583379
C	0.000000	-0.758913	0.583379
O	0.559888	-1.330523	-0.596157
H	1.352955	-0.831182	-0.833514
H	-1.352955	0.831182	-0.833514
H	-1.023394	-1.137436	0.624543
H	1.023394	1.137436	0.624543
H	-0.522816	1.107511	1.481317
H	0.522816	-1.107511	1.481317

Vibrational Frequencies

122.3840	132.3677	304.0922
321.6963	538.6583	893.4859
905.7835	1069.8927	1098.1831
1158.7543	1174.7897	1311.7004
1334.9227	1388.7990	1444.5549
1466.7400	1556.4887	1558.8055
3086.2062	3097.5983	3159.3728
3179.3413	3864.9789	3865.5208

g+Tg-

Cartesian Coordinates

H	-2.023610	-0.663982	0.648970
O	-1.843871	-0.100198	-0.114260
C	-0.562230	0.508454	0.065494
C	0.562208	-0.508392	-0.065447
O	1.843899	0.100146	0.114218
H	2.023641	0.663847	-0.649078
H	0.486414	-1.016909	-1.029983
H	0.485622	-1.258897	0.721142
H	-0.485602	1.259024	-0.721044
H	-0.486550	1.016960	1.030043

Vibrational Frequencies

147.2574	261.6285	297.2232
312.2566	478.7627	814.9045
1034.5287	1076.0478	1096.6942
1119.9310	1138.6859	1334.6539
1350.5064	1376.1565	1416.4481
1463.3164	1551.9132	1564.3061
3118.2315	3125.3231	3186.1077
3209.7030	3877.8678	3879.1576

G+Tg+

Cartesian Coordinates

H	0.329965	2.042194	0.757585
O	0.706966	1.709624	-0.067195
C	0.706966	0.281140	-0.024685
C	-0.706966	-0.281140	-0.024685
O	-0.706966	-1.709624	-0.067195
H	-0.329965	-2.042194	0.757585
H	-1.230856	0.045717	-0.919752
H	-1.259291	0.086895	0.847834
H	1.230856	-0.045717	-0.919752
H	1.259291	-0.086895	0.847834

Vibrational Frequencies

152.6955	270.9072	274.7900
324.6648	479.3539	816.6710
1048.0571	1055.6819	1094.6608
1116.9214	1160.3573	1313.0507
1360.2744	1392.2993	1400.5743
1463.3121	1552.2160	1564.3656
3087.0163	3090.4060	3213.9281
3229.2309	3874.2894	3875.2924

tG+g-

Cartesian Coordinates

C	0.727372	0.574059	0.276055
H	0.688219	0.587574	1.369790
H	1.287714	1.443497	-0.064765
C	-0.680186	0.610604	-0.271778
H	-0.649135	0.606679	-1.363877
H	-1.202203	1.506928	0.075941
O	-1.321930	-0.577251	0.220015
H	-2.144605	-0.717576	-0.264178
O	1.430381	-0.572789	-0.193713
H	0.869278	-1.334758	0.011012

Vibrational Frequencies

177.5247	258.1977	336.2267
451.8472	534.3804	896.7512
914.8321	1070.0350	1106.9481
1137.4538	1181.7129	1278.4035
1305.2084	1395.4443	1436.6473
1478.2118	1545.1240	1555.2832
3101.6339	3109.2848	3168.6538
3205.3811	3849.0586	3895.3685

tG+g+

Cartesian Coordinates

C	0.686913	0.539693	0.306815
H	0.611948	0.472302	1.399258
H	1.178650	1.487319	0.058649
C	-0.698473	0.546313	-0.300095
H	-0.617581	0.511350	-1.384813
H	-1.196600	1.480951	-0.016998
O	-1.488951	-0.583496	0.058458
H	-1.537185	-0.631702	1.021949
O	1.408803	-0.569330	-0.224122
H	2.271315	-0.613648	0.206947

Vibrational Frequencies

129.8847	233.1696	257.5783
338.1240	518.9413	896.7964
910.4271	1065.8172	1103.6662
1140.1553	1199.4697	1263.5981
1330.4183	1386.2094	1441.6957
1487.1426	1539.2371	1558.7887
3065.8743	3091.7289	3121.6132
3213.6141	3873.4004	3885.0403

tG+t

Cartesian Coordinates

O	0.286653	-1.413362	-0.565234
C	-0.286653	-0.696561	0.529231
C	0.286653	0.696561	0.529231
O	-0.286653	1.413362	-0.565234
H	-0.076184	-2.307601	-0.571745
H	0.076184	2.307601	-0.571745
H	1.374435	0.633236	0.436770
H	-1.374435	-0.633236	0.436770
H	-0.036550	-1.176727	1.481455
H	0.036550	1.176727	1.481455

Vibrational Frequencies

145.0079	204.5265	217.0053
352.7436	499.4979	906.2736
922.4893	1083.8823	1099.5703
1139.0396	1240.9352	1244.1322
1291.4722	1342.6166	1447.0676
1511.8699	1550.7326	1551.3352
3082.7047	3094.1364	3147.2186
3159.0356	3887.9311	3888.2043

tTg+

Cartesian Coordinates

H	-2.523511	0.355875	-0.102272
O	-1.781466	-0.240566	0.054930
C	-0.562433	0.501678	-0.042945
C	0.566419	-0.511104	-0.001177
O	1.841383	0.131612	-0.084196
H	2.006656	0.591524	0.748532
H	0.504980	-1.167737	-0.865665
H	0.479961	-1.120134	0.902072
H	-0.506569	1.065579	-0.977116
H	-0.464768	1.203082	0.793305

Vibrational Frequencies

129.7662	212.1165	271.4920
305.6610	482.3228	832.1621
1028.9872	1082.0696	1087.7697
1108.4913	1221.7467	1248.9592
1333.1527	1374.5016	1405.4279
1488.2121	1559.5612	1573.8459
3085.1798	3127.6777	3156.7995
3227.8143	3880.4723	3891.1732

tTt

Cartesian Coordinates

H	-0.089377	2.547653	0.000000
O	0.440950	1.741775	0.000000
C	-0.440950	0.613808	0.000000
C	0.440950	-0.613808	0.000000
O	-0.440950	-1.741775	0.000000
H	0.089377	-2.547653	0.000000
H	1.076180	-0.603938	0.888944
H	1.076180	-0.603938	-0.888944
H	-1.076180	0.603938	0.888944
H	-1.076180	0.603938	-0.888944

Vibrational Frequencies

95.2583	178.8793	209.7759
299.0001	484.5511	851.1230
1014.7030	1078.3001	1098.5078
1184.4237	1188.2893	1242.4669
1293.6985	1327.9870	1415.2005
1511.8768	1573.4357	1580.7738
3108.4418	3113.1575	3159.8746
3183.9782	3894.1732	3894.9686

Ethylene Glycol complexes with 1 water**1**

Cartesian Coordinates

C	0.822798	0.796353	0.521799
C	1.310611	-0.609438	0.216384
H	1.670655	1.417886	0.816584
O	0.233626	1.382449	-0.639529
H	0.104252	0.774786	1.343271
O	0.252377	-1.422842	-0.324486
H	2.140266	-0.573177	-0.492964
H	1.646437	-1.109034	1.124898
H	0.148097	-1.146611	-1.246282
H	-0.721991	1.224148	-0.575337
O	-2.136260	-0.028836	0.243046
H	-3.039348	-0.352652	0.157854
H	-1.546767	-0.803000	0.210625

Vibrational Frequencies

102.9890	148.2459	160.2331
181.9057	201.1388	305.3022
361.9879	400.6003	527.5515
552.0625	753.8522	888.3900
906.0948	1062.3872	1089.8785
1133.7400	1220.6900	1290.0601
1404.5371	1425.3332	1427.8960
1451.3733	1539.1763	1544.2660
1636.1626	3124.1737	3128.6021
3189.5095	3208.6633	3719.7177
3799.8454	3855.5681	3966.0353

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Cartesian Coordinates

C	1.357177	-0.531263	0.172676
C	0.749597	0.813225	0.537138
H	1.816080	-0.946304	1.078110
O	0.437014	-1.442055	-0.409700
H	2.151969	-0.394798	-0.564907
O	-0.023208	1.392879	-0.528381
H	0.048988	0.707736	1.364168
H	1.545883	1.497379	0.844878
H	0.454963	1.263487	-1.359234
H	-0.444469	-1.305456	-0.020176
O	-2.105484	-0.268644	0.279096
H	-2.967504	-0.443755	-0.113662
H	-1.713130	0.472500	-0.216172

Vibrational Frequencies

93.9391	158.0633	164.0140
214.9937	253.8084	305.5076
319.9812	394.3053	488.2655
549.3667	735.6605	891.1654
900.6162	1087.5598	1098.9626
1157.8031	1208.4223	1307.3689
1352.3723	1404.6802	1456.4135
1482.2806	1557.3264	1561.5784
1646.5939	3083.1699	3116.8291
3151.2116	3208.1467	3711.6154
3751.9564	3862.2313	3963.3481

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Cartesian Coordinates

C	0.373516	0.659302	-1.301931
C	-0.373516	-0.659302	-1.301931
H	0.126043	1.224690	-2.200948
O	0.000000	1.492632	-0.202237
H	1.450602	0.465452	-1.295546
O	0.000000	-1.492632	-0.202237
H	-1.450602	-0.465452	-1.295546
H	-0.126043	-1.224690	-2.200948
H	-0.296977	-1.070634	0.617351
H	0.296977	1.070634	0.617351
O	0.000000	0.000000	2.345745
H	0.654866	-0.407821	2.925645
H	-0.654866	0.407821	2.925645

Vibrational Frequencies

27.9348	115.0774	134.4657
183.9442	184.9252	270.1694
295.3761	347.9958	522.7465
541.1681	578.9259	883.4834
904.7871	1074.3161	1117.8976
1136.5443	1231.1921	1264.5028
1398.2147	1423.8803	1428.4633
1456.0911	1535.6715	1538.5825
1642.1568	3104.5458	3108.4078
3189.1792	3191.8210	3824.4118
3834.7086	3855.7844	3990.3138

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Cartesian Coordinates

C	0.447588	0.902486	0.597731
C	0.955812	-0.520218	0.613876
H	1.288452	1.600216	0.621017
O	-0.350943	1.137449	-0.570592
H	-0.196063	1.089102	1.455329
O	1.735908	-0.662955	-0.586506
H	1.574445	-0.689659	1.499738
H	0.112555	-1.212575	0.615001
H	1.826197	-1.601363	-0.792733
H	0.191304	0.847783	-1.320990
O	-2.391212	-0.709414	0.042132
H	-1.857218	0.029670	-0.300083
H	-3.310093	-0.477416	-0.127194

Vibrational Frequencies

42.9287	78.9620	142.4519
169.3331	217.6171	283.4917
339.0334	383.4494	501.7186
544.5597	715.2890	900.5406
916.3674	1066.9623	1100.8298
1130.1953	1189.1177	1285.0366
1308.7947	1394.6509	1438.4219
1481.2697	1543.7386	1561.4700
1651.9251	3110.4688	3127.4423
3188.4435	3219.5279	3703.6190
3825.7618	3894.7717	3964.6332

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Cartesian Coordinates

C	1.371087	0.530710	-0.079711
C	0.917852	-0.813750	0.447233
H	1.735701	0.411960	-1.101934
O	0.249598	1.440280	-0.055162
H	2.172175	0.923267	0.553916
O	0.067679	-1.504083	-0.455273
H	1.802545	-1.437118	0.586613
H	0.439442	-0.676407	1.422229
H	-0.834255	-1.158886	-0.335301
H	0.500959	2.255865	-0.506982
O	-2.197086	0.093968	0.190378
H	-2.962654	0.326075	-0.346067
H	-1.549071	0.812158	0.082852

Vibrational Frequencies

61.7421	146.0383	191.0986
221.5570	258.5215	262.1260
341.6806	391.1863	497.5276
521.9444	736.5305	882.8084
916.2131	1074.5086	1119.1781
1138.2538	1216.2093	1283.0472
1334.5896	1430.3360	1470.5808
1476.5343	1531.2389	1546.1353
1652.1886	3101.9080	3107.8816
3175.2924	3184.8559	3714.2876
3756.9640	3884.0163	3965.9052

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Cartesian Coordinates

C 0.211820 0.725049 -0.227271
 C 1.704859 0.488321 -0.142943
 H -0.184078 0.343542 -1.174408
 O -0.448318 0.084323 0.871647
 H -0.020721 1.787035 -0.158694
 O 1.974313 -0.920447 -0.067943
 H 2.220059 0.949719 -0.989449
 H 2.100531 0.904005 0.781692
 H 1.864307 -1.304511 -0.948346
 H -0.005210 -0.772214 0.985689
 O -2.964540 -0.268638 -0.385433
 H -3.755018 -0.194547 0.158725
 H -2.211591 -0.155156 0.219910

Vibrational Frequencies

23.2714 51.5072 122.1847
 166.5103 199.1985 325.6797
 346.5211 380.6247 503.2904
 558.6621 715.7975 890.1409
 908.1817 1072.1943 1075.3774
 1122.1406 1215.6833 1251.1986
 1381.5542 1388.1499 1427.2327
 1466.5319 1543.4602 1556.1545
 1655.8480 3104.6891 3125.3452
 3201.2214 3220.2841 3723.3536
 3806.6057 3866.9691 3968.6080

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Cartesian Coordinates

C 0.316983 0.696263 0.736237
 O -0.352209 1.152304 -0.447280
 C 0.968863 -0.646098 0.477961
 O 1.860562 -0.545063 -0.646787
 O -2.473024 -0.654443 -0.044128
 H 1.063926 1.434232 1.047599
 H -0.443232 0.614919 1.511596
 H 1.490980 -1.004261 1.368990
 H 0.213734 -1.374310 0.190198
 H 2.693163 -0.155966 -0.348451
 H 0.262650 0.989853 -1.180520
 H -1.920673 0.072895 -0.379413
 H -3.358262 -0.500738 -0.389623

Vibrational Frequencies

42.9877 73.0993 130.6592
 162.5245 221.3746 297.5825
 339.1014 398.0700 497.3068
 544.9488 692.2439 892.4953
 905.1717 1068.6554 1072.8617
 1117.2691 1210.4945 1253.1953
 1381.4828 1385.3819 1426.5961
 1462.4790 1546.0309 1549.6076
 1650.5553 3100.3892 3126.1940
 3208.7998 3229.2575 3723.5935
 3813.5998 3873.4408 3968.0628

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Cartesian Coordinates

C 1.345915 0.565941 -0.102109
 O 0.205365 1.448941 -0.012567
 C 0.958196 -0.789896 0.448139
 O 0.105957 -1.522069 -0.416512
 O -2.220333 0.069328 0.005536
 H 1.653956 0.454678 -1.143178
 H 2.170772 0.981558 0.484242
 H 1.867635 -1.381493 0.562312
 H 0.512770 -0.659430 1.440461
 H -0.798386 -1.174252 -0.323463
 H 0.373076 2.228894 -0.556843
 H -1.545786 0.768759 0.068730
 H -2.786616 0.155408 0.779904

Vibrational Frequencies

73.5813 149.6252 195.9041
 236.0886 249.4552 266.1884
 333.5966 344.7165 505.3419
 662.1978 743.2920 881.1942
 921.0704 1074.9671 1115.7706
 1138.9844 1213.8041 1289.9697
 1331.2957 1427.8970 1457.9813
 1475.1983 1531.9539 1545.4056
 1638.7906 3098.0921 3105.9856
 3179.5125 3185.3621 3704.5631
 3751.2375 3884.5906 3963.9231

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Cartesian Coordinates

C	-1.174332	-0.692523	0.348205
O	-0.204293	-1.554551	-0.221282
C	-1.217671	0.678052	-0.302952
O	-0.065176	1.488287	0.014971
O	2.235422	-0.072820	0.113136
H	-2.139395	-1.178752	0.195472
H	-1.025105	-0.578452	1.429945
H	-1.202721	0.569497	-1.385358
H	-2.129284	1.207895	-0.011286
H	-0.157088	1.798311	0.926126
H	0.686189	-1.209614	-0.029450
H	1.652638	0.675695	-0.106883
H	2.939160	-0.085092	-0.544679

Vibrational Frequencies

74.0043	131.7666	187.5544
222.6540	256.2400	312.9007
346.6321	431.9297	525.5982
569.5322	784.2971	869.8823
917.3814	1069.9601	1090.1503
1144.9866	1212.6134	1291.3610
1396.1419	1422.0274	1438.9818
1467.4963	1533.8889	1534.8479
1632.3150	3071.1272	3115.4510
3174.2580	3222.4249	3697.8891
3742.1070	3868.5829	3962.7474

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Cartesian Coordinates

C	-0.387001	0.714652	0.710777
O	0.322145	1.022306	-0.512993
C	-1.048308	-0.624801	0.487877
O	-2.000933	-0.560863	-0.570957
O	2.594425	-0.604198	0.038248
H	0.314006	0.665759	1.547319
H	-1.144095	1.477033	0.900338
H	-0.281207	-1.377836	0.287447
H	-1.599060	-0.917874	1.380369
H	-1.529681	-0.223157	-1.345413
H	0.499549	1.971347	-0.543404
H	1.911799	-0.040116	-0.360500
H	3.115445	-0.952215	-0.692458

Vibrational Frequencies

26.5280	42.6842	110.5084
158.1586	210.3342	288.3699
333.1459	382.3597	430.9762
530.5396	661.1611	890.1929
916.3918	1058.8731	1104.2996
1130.6264	1184.3742	1288.8042
1307.6224	1396.1543	1434.5637
1476.5264	1547.6833	1550.4823
1648.3550	3120.7215	3123.7695
3192.0554	3211.1024	3751.1056
3859.2170	3885.2285	3972.4087

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Cartesian Coordinates

C	-0.286241	0.708565	-0.247312
O	0.452223	-0.068655	0.721423
C	-1.770984	0.467021	-0.081239
O	-2.087024	-0.911717	-0.236557
O	3.144395	-0.112930	-0.275417
H	-0.041898	1.769608	-0.157710
H	0.049959	0.346422	-1.216317
H	-2.100298	0.835024	0.898440
H	-2.327372	1.002430	-0.850146
H	-1.465070	-1.403706	0.318884
H	0.393768	0.370427	1.581548
H	2.260864	-0.225846	0.110753
H	3.496643	-1.001453	-0.389746

Vibrational Frequencies

22.7088	36.7218	123.3235
154.2908	189.1673	289.2417
342.1628	389.5258	468.2817
548.0128	660.7923	887.6636
906.0575	1062.2651	1081.4817
1127.3494	1207.7503	1255.7331
1384.9508	1388.4808	1427.8573
1461.4624	1541.5724	1550.3012
1648.3650	3079.8941	3133.4159
3194.7210	3229.5013	3759.9031
3846.3532	3861.9615	3971.9013

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Cartesian Coordinates

C	-1.370462	-0.553677	-0.159030
O	-0.274462	-1.454828	0.038791
C	-1.005811	0.778894	0.441616
O	-0.027297	1.399313	-0.404186
O	2.443806	-0.138071	0.084683
H	-1.580147	-0.418379	-1.222712
H	-2.268265	-0.932430	0.338793
H	-1.905282	1.398290	0.499026
H	-0.608992	0.626224	1.448702
H	0.192987	2.264225	-0.033010
H	-0.400366	-2.223518	-0.531821
H	1.737633	0.413504	-0.285150
H	1.953702	-0.930531	0.336345

Vibrational Frequencies

33.3914	81.6599	136.8651
180.1964	203.0271	228.5145
287.3533	347.4624	404.1095
505.0418	640.0998	904.0827
919.7138	1083.0492	1096.7946
1131.2754	1240.5701	1257.6240
1305.7216	1345.6412	1446.9553
1508.9265	1548.9276	1550.5438
1688.3871	3098.9559	3107.7989
3163.6028	3173.7392	3811.4747
3872.8138	3885.6543	3942.1063

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Cartesian Coordinates

C	-1.374649	-0.536195	0.049161
O	-0.399157	-1.504523	-0.310204
C	-0.805613	0.788945	0.506173
O	-0.000320	1.353661	-0.550422
O	2.132271	-0.243749	0.270781
H	-2.001439	-0.378089	-0.829058
H	-2.008535	-0.913110	0.860770
H	-1.634343	1.458607	0.748751
H	-0.189890	0.652809	1.400085
H	0.095765	2.300296	-0.382510
H	0.442256	-1.308203	0.134410
H	2.862756	-0.572231	-0.264984
H	1.652649	0.400318	-0.280713

Vibrational Frequencies

73.2162	143.3041	162.7682
230.6099	244.9053	285.1921
325.5594	399.0389	447.7784
522.0876	769.5507	886.4075
902.1781	1083.4892	1130.4020
1144.7462	1235.3400	1271.3986
1343.9337	1392.6410	1453.8987
1495.9310	1552.0828	1555.3278
1645.9521	3084.3357	3106.1663
3164.3468	3183.8811	3706.0052
3769.3981	3878.3340	3958.6088

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Cartesian Coordinates

C	-0.520726	0.916800	-0.293953
C	-0.911863	-0.402336	0.334802
H	-1.264718	1.674886	-0.043124
O	0.765798	1.274063	0.249314
H	-0.466133	0.809092	-1.378571
O	-2.234344	-0.680664	-0.139189
H	-0.204513	-1.177799	0.037715
H	-0.895633	-0.303297	1.423423
H	-2.430697	-1.609925	0.029667
H	1.028093	2.127246	-0.119789
O	2.423487	-1.013840	-0.186511
H	1.994762	-0.168803	0.030380
H	3.194849	-1.074655	0.386296

Vibrational Frequencies

42.7702	60.4814	119.8585
128.6528	195.6816	205.8330
292.9000	303.8827	372.5308
483.0192	667.4113	851.5001
1015.1733	1070.3268	1093.7063
1173.7410	1206.6865	1254.3324
1301.9981	1339.8256	1421.6524
1513.1277	1570.9544	1583.8066
1657.3010	3113.8310	3126.4972
3178.7748	3201.4813	3737.9535
3883.6228	3897.1814	3968.2335

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Cartesian Coordinates

C	-0.458775	0.876914	-0.368172
C	-0.932602	-0.359657	0.372359
H	-1.204962	1.669572	-0.289649
O	0.816470	1.326595	0.126211
H	-0.304122	0.647424	-1.419352
O	-2.229608	-0.662480	-0.153051
H	-0.226679	-1.175440	0.211824
H	-0.990361	-0.150407	1.446438
H	-2.439739	-1.580751	0.055007
H	0.690493	1.710295	1.004164
O	2.362110	-1.050506	-0.042065
H	2.014430	-0.143321	-0.002639
H	3.217430	-0.989778	-0.479672

Vibrational Frequencies

59.1563	69.9367	122.1919
152.7369	201.3242	213.4479
287.0942	309.4620	397.3019
485.9964	676.0489	830.7154
1028.6602	1080.2237	1087.2709
1100.3022	1217.8465	1266.8897
1342.0895	1373.9424	1406.3606
1492.1065	1557.4564	1577.5209
1649.3449	3088.2521	3143.1692
3182.7634	3236.5079	3733.7821
3875.2578	3896.4903	3968.0377

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Cartesian Coordinates

C	0.351122	0.802187	-0.467233
C	1.005405	-0.182782	0.490618
H	0.035011	0.292581	-1.375510
O	-0.855178	1.358817	0.089894
H	1.054679	1.592286	-0.735997
O	2.182231	-0.747491	-0.094105
H	1.341716	0.333847	1.390450
H	0.285895	-0.951237	0.777561
H	1.909002	-1.440027	-0.709344
H	-0.622470	1.898404	0.857394
O	-2.200811	-1.121426	-0.022764
H	-3.141211	-1.186642	-0.218260
H	-2.011722	-0.174844	0.089203

Vibrational Frequencies

50.5044	78.8814	129.0275
149.8712	207.1900	258.9989
288.9487	333.4047	374.2556
479.4096	633.6733	814.3007
1036.1418	1064.6754	1094.4308
1113.4795	1146.7102	1334.9036
1351.2288	1386.1487	1415.9802
1467.2034	1550.6475	1562.5568
1647.4886	3132.3052	3140.4139
3197.4388	3225.6661	3747.5132
3870.6004	3879.9639	3969.7870

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Cartesian Coordinates

C	-0.503118	0.815806	-0.369672
C	-1.095895	-0.340846	0.422475
H	-1.213530	1.643334	-0.409970
O	0.668688	1.329337	0.256377
H	-0.306415	0.488358	-1.394843
O	-2.285528	-0.852020	-0.190773
H	-0.397122	-1.175729	0.442158
H	-1.281875	-0.020471	1.451345
H	-2.965794	-0.167994	-0.142221
H	1.371321	0.666878	0.154461
O	2.621195	-0.776531	-0.103325
H	3.304127	-0.719180	-0.781991
H	3.048532	-1.171242	0.666009

Vibrational Frequencies

34.5653	56.5566	79.2495
142.8682	187.8466	204.3975
241.6949	279.0647	321.0889
481.2105	705.1901	817.4721
1043.1411	1085.1549	1105.3253
1121.6494	1169.0521	1339.4060
1351.6119	1391.3645	1448.2589
1461.9985	1551.7085	1564.1396
1642.4562	3106.4664	3118.8035
3174.4313	3211.8370	3781.9785
3857.8687	3874.0282	3997.0935

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Cartesian Coordinates

C	-1.038690	-0.133646	0.514090
C	-0.335293	0.800470	-0.453625
H	-1.442267	0.432119	1.351134
O	-2.155577	-0.761599	-0.120139
H	-0.327314	-0.868604	0.894048
O	0.819941	1.325778	0.232934
H	-0.022141	0.250895	-1.345268
H	-1.009900	1.605429	-0.748456
H	1.127515	2.112514	-0.235318
H	-1.821405	-1.470163	-0.685006
O	2.184471	-1.125407	-0.123918
H	2.990778	-1.354084	0.349718
H	1.957956	-0.219225	0.145339

Vibrational Frequencies

45.0554	66.4181	130.9778
143.5735	212.1322	275.4002
292.4107	301.3127	394.7334
481.2132	657.8968	829.5662
1037.9160	1059.3754	1081.7283
1112.2677	1214.2200	1270.0099
1337.5417	1391.2198	1403.6789
1485.5388	1557.5502	1567.0360
1651.6867	3115.0677	3145.1336
3183.8016	3227.6099	3737.5522
3878.9196	3884.7641	3969.5521

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Cartesian Coordinates

C	0.298965	-0.154420	-0.273312
C	1.620949	0.367798	0.254162
H	0.012266	-1.058024	0.258815
O	-0.752557	0.796621	-0.034377
H	0.384623	-0.389376	-1.335523
O	2.596116	-0.630546	-0.053612
H	1.866073	1.318887	-0.231056
H	1.540195	0.537247	1.330528
H	3.426601	-0.401777	0.381333
H	-0.674816	1.516919	-0.673734
O	-3.325046	-0.478159	0.021394
H	-3.744485	-0.304038	0.870048
H	-2.478037	-0.003441	0.047254

Vibrational Frequencies

23.3425	32.6539	106.0618
135.7670	168.2330	205.9139
275.2621	297.8293	392.8262
489.3358	669.2828	831.9313
1030.7148	1084.5129	1092.9328
1102.7046	1220.4803	1251.4029
1332.7881	1375.3024	1406.9237
1491.3307	1558.9724	1574.7546
1653.9525	3088.5293	3144.9981
3158.4359	3236.5491	3754.1566
3877.8991	3890.7285	3971.0533

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Cartesian Coordinates

C	-0.258954	-0.167731	0.085525
C	-1.651629	0.411141	-0.107685
H	-0.041141	-0.882629	-0.703782
O	0.748030	0.852681	-0.018865
H	-0.183105	-0.684314	1.047307
O	-2.646423	-0.612778	-0.094544
H	-1.854877	1.170889	0.655699
H	-1.720040	0.884175	-1.084448
H	-2.691338	-0.990573	0.793355
H	0.662789	1.453360	0.733977
O	3.272468	-0.507294	0.046421
H	2.468972	0.027244	-0.062783
H	3.829642	-0.299483	-0.710462

Vibrational Frequencies

25.7409	32.9274	121.3441
152.8664	166.0654	280.3070
283.7863	310.6583	416.7848
485.2529	671.9363	816.3705
1049.1863	1058.3318	1090.6330
1116.6413	1162.2889	1313.5066
1361.6420	1393.9591	1402.7726
1466.5412	1552.7724	1564.5274
1651.2779	3091.5963	3112.7074
3217.1110	3235.5691	3753.3618
3868.4011	3874.9426	3971.6373

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Cartesian Coordinates

C	-0.472428	0.859257	-0.372867
C	-0.954638	-0.375371	0.375653
H	-1.213313	1.662441	-0.312130
O	0.798627	1.319920	0.118595
H	-0.314809	0.617005	-1.420909
O	-2.195144	-0.841658	-0.159386
H	-0.241874	-1.186267	0.249366
H	-1.042366	-0.156802	1.446047
H	-2.888101	-0.208494	0.067867
H	0.681670	1.659098	1.016217
O	2.432550	-1.007113	-0.023050
H	2.045207	-0.116124	-0.021332
H	3.247709	-0.943367	-0.531107

Vibrational Frequencies

50.7004	60.0676	124.2222
152.4679	201.5052	267.2890
276.1580	308.2050	402.1486
481.2471	664.4960	817.0981
1046.7805	1055.6522	1086.9288
1112.5207	1159.8759	1320.4322
1360.7378	1394.9042	1401.8090
1466.3907	1552.2775	1565.5577
1644.7466	3091.7877	3110.3401
3222.7517	3238.0287	3746.4990
3870.7617	3875.3975	3970.3120

Ethylene Glycol + 2 Water Complexes

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Cartesian Coordinates

C	1.870795	0.183971	0.275838
C	0.871783	-0.874305	0.717210
H	2.752386	-0.281719	-0.163708
O	1.302652	0.985756	-0.758745
H	2.182181	0.785073	1.134866
H	0.083001	-0.414447	1.318181
O	0.279831	-1.495001	-0.439155
H	0.507395	1.428331	-0.399243
H	1.356317	-1.653647	1.305883
H	0.449298	-0.873471	-1.170514
O	-2.360837	-0.732324	-0.153088
H	-2.962348	-1.291712	0.349599
H	-1.531253	-1.240277	-0.273534
O	-1.198035	1.764669	0.317246
H	-1.717138	2.521707	0.023990
H	-1.764190	0.977359	0.186131

Vibrational Frequencies

64.3268	87.4099	115.7866
175.1129	204.8543	211.4138
219.6658	237.0162	263.0294
333.3915	390.8957	453.9613
563.8032	625.2055	718.4928
770.4642	882.3595	900.0038
913.8659	1085.0845	1121.0687
1133.5688	1244.7558	1262.4913
1366.6643	1413.9262	1462.1883
1484.5563	1550.6754	1568.1040
1662.1539	1691.2026	3114.6909
3123.5864	3187.3683	3204.1360
3576.9206	3633.6678	3666.1960
3740.2533	3951.6934	3958.1543

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Cartesian Coordinates

C	-0.220376	0.728021	1.293893
C	0.220376	-0.728021	1.293893
H	0.216176	1.238057	2.154321
O	0.220376	1.419847	0.113991
H	-1.307022	0.793155	1.364578
H	-0.216176	-1.238057	2.154321
O	-0.220376	-1.419847	0.113991
H	-0.510887	1.346719	-0.526103
H	1.307022	-0.793155	1.364578
H	0.510887	-1.346719	-0.526103
O	2.035443	-0.285414	-1.117630
H	2.498201	-0.062837	-1.932307
H	1.602940	0.530571	-0.794734
O	-2.035443	0.285414	-1.117630
H	-1.602940	-0.530571	-0.794734
H	-2.498201	0.062837	-1.932307

Vibrational Frequencies

68.3448	143.4113	170.4446
174.2230	183.3945	196.4079
226.6231	234.1602	250.2436
328.8922	433.9266	445.3540
521.0636	553.2385	648.0555
704.2609	875.3217	886.9738
926.7138	1073.4984	1104.6728
1134.6556	1252.1149	1304.6142
1426.3192	1448.5498	1458.3891
1458.4221	1539.1471	1543.6865
1651.0756	1653.8021	3129.2314
3134.7002	3192.7072	3207.8629
3618.5797	3635.6437	3728.2999
3737.8312	3960.6210	3960.8172

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Cartesian Coordinates

C	0.877812	-0.367448	0.794082
C	2.136192	0.389605	0.423118
H	0.408411	0.062649	1.683079
O	-0.036884	-0.362473	-0.315278
H	1.114670	-1.413586	0.982099
H	2.872073	0.325142	1.224591
O	2.742758	-0.175501	-0.735829
H	-0.486980	0.505614	-0.337185
H	1.894837	1.446450	0.259461
H	2.027078	-0.300789	-1.376724
O	-2.697911	-1.131371	0.021060
H	-1.739479	-1.216071	-0.144345
H	-3.130767	-1.843440	-0.461512
O	-2.006612	1.570903	-0.040115
H	-2.619761	0.813470	-0.033128
H	-2.434909	2.275150	-0.538243

Vibrational Frequencies

33.0036	40.4715	75.2138
126.2161	177.2844	191.3363
197.9823	232.2841	243.0096
347.2097	365.8057	451.4820
465.0541	544.7181	559.2442
703.1152	870.7212	901.5277
914.3624	1073.7999	1123.2381
1129.6791	1224.0653	1272.9067
1386.9178	1420.5636	1447.6439
1463.2071	1539.9198	1551.9865
1643.4854	1665.1591	3088.0891
3121.3160	3190.5772	3211.4987
3638.3462	3686.6605	3727.0757
3836.1341	3963.5052	3965.7716

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Cartesian Coordinates

C	-1.564777	-0.751459	0.387943
C	-1.384738	0.201655	-0.773680
H	-2.038187	-1.663978	0.006229
O	-0.353021	-1.040724	1.069633
H	-2.227918	-0.303803	1.127315
H	-2.353443	0.367324	-1.253697
O	-0.869782	1.448304	-0.261607
H	0.294412	-1.373412	0.422567
H	-0.685779	-0.217368	-1.501466
H	-0.861864	2.092258	-0.982624
O	1.706282	-1.125505	-0.884950
H	2.501778	-1.612622	-1.124946
H	1.996344	-0.297869	-0.447101
O	1.811034	1.217419	0.591242
H	1.863092	0.985815	1.526514
H	0.852552	1.326523	0.427084

Vibrational Frequencies

47.6787	88.8487	111.6385
166.3185	178.1893	221.1941
222.0953	241.8922	255.8426
335.0872	356.5524	406.2162
481.5268	528.3428	671.2523
805.1454	856.4303	894.1511
917.5715	1086.6898	1115.4198
1138.8076	1234.2900	1260.0105
1344.7983	1419.7171	1457.4419
1489.1732	1541.0431	1555.9374
1664.2938	1684.5740	3085.7408
3107.4429	3170.7970	3199.4773
3582.4579	3656.6355	3732.8480
3871.0516	3934.6143	3956.3163

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Cartesian Coordinates

C	-2.161581	0.324162	0.469452
C	-0.898178	-0.451532	0.760989
H	-1.936881	1.396444	0.472071
O	-2.727110	-0.071187	-0.777125
H	-2.913829	0.125899	1.231789
H	-1.114321	-1.521558	0.780948
O	0.010922	-0.155627	-0.312283
H	-1.997345	-0.061553	-1.413866
H	-0.470642	-0.149746	1.721830
H	0.738519	-0.808138	-0.305588
O	2.218134	1.519803	0.039573
H	2.365119	2.333744	-0.453676
H	1.298197	1.243517	-0.135171
O	2.542804	-1.255961	-0.037750
H	3.182351	-1.759226	-0.552673
H	2.849384	-0.331394	-0.027631

Vibrational Frequencies

28.7763	40.5021	74.1033
127.8120	185.6991	191.6605
197.5088	230.6746	234.7122
345.5521	369.2681	445.1984
468.0442	541.5420	555.8627
698.4203	868.3300	898.6148
920.0499	1074.6674	1127.8076
1145.9909	1216.0399	1283.8252
1359.2864	1390.1799	1441.5677
1489.3215	1547.4521	1554.1364
1644.9621	1664.6584	3096.6195
3105.9658	3176.0487	3201.6602
3643.6720	3691.1680	3733.4944
3841.8843	3962.5112	3967.2432

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Cartesian Coordinates

C	-1.934533	-0.463626	-0.225009
C	-0.598888	-1.170016	-0.183672
H	-2.490386	-0.676227	0.690068
O	-1.692767	0.956942	-0.338596
H	-2.505137	-0.807169	-1.092257
H	0.002095	-0.865807	-1.046039
O	0.106289	-0.960109	1.035902
H	-2.529749	1.426016	-0.229254
H	-0.772873	-2.243841	-0.250742
H	0.389395	-0.031299	1.063685
O	2.804774	-0.507039	-0.569490
H	2.353718	0.339150	-0.439216
H	2.392925	-1.087393	0.083390
O	0.931179	1.692105	0.256278
H	0.012280	1.755206	-0.062261
H	1.152456	2.538027	0.661957

Vibrational Frequency

32.6049	71.3516	77.8603
123.5447	150.8693	202.8045
207.1804	236.3510	263.6538
303.1873	345.1797	354.0376
386.3475	510.9015	526.9723
585.9631	680.4165	884.0598
912.3667	1070.7781	1120.7888
1134.7512	1211.8322	1284.0007
1325.9074	1425.2684	1451.0961
1480.3395	1537.4735	1547.9695
1656.9848	1681.1642	3109.8230
3116.6027	3181.7648	3199.2170
3707.3406	3780.8220	3822.1969
3884.9290	3946.6617	3956.5789

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Cartesian Coordinates

C	-1.510221	-0.231114	0.745139
C	-1.237343	-1.045064	-0.505873
H	-0.774226	-0.467283	1.511511
O	-1.378429	1.183803	0.520468
H	-2.508121	-0.462563	1.130199
H	-1.909065	-0.725202	-1.311274
O	0.119591	-0.974200	-0.932041
H	-2.117880	1.479266	-0.027640
H	-1.438251	-2.097330	-0.300380
H	0.354637	-0.041071	-1.121578
O	1.215336	1.598262	-0.688474
H	0.481404	1.821114	-0.095097
H	1.873378	1.164950	-0.120558
O	2.275533	-0.646562	0.824755
H	3.052466	-1.215632	0.840853
H	1.614800	-1.089608	0.260696

Vibrational Frequencies

45.0546	70.0313	130.2926
152.2890	173.4799	199.1938
223.6307	233.2897	307.7510
344.5049	358.5662	464.5531
505.5375	536.6692	566.5289
678.9594	856.2179	893.2631
915.7894	1072.4507	1093.1562
1144.2767	1219.0421	1294.5606
1390.9131	1421.6663	1443.3182
1475.5016	1536.6231	1539.6481
1640.4943	1689.7672	3086.9401
3111.9383	3183.1730	3216.8147
3593.2202	3692.8231	3764.7235
3868.6124	3879.3215	3960.7262

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Cartesian Coordinates

C	0.476089	1.287550	0.647596
C	-0.307486	1.336020	-0.657106
H	0.231539	2.181982	1.229218
O	0.246234	0.104317	1.419865
H	1.547273	1.298034	0.446064
H	0.070368	2.171048	-1.255211
O	-0.263130	0.117910	-1.407509
H	-0.683521	-0.176456	1.331571
H	-1.363851	1.517449	-0.456269
H	0.612564	-0.302218	-1.297714
O	1.955864	-1.211557	-0.282119
H	1.440409	-1.056006	0.534435
H	2.169244	-2.150761	-0.304448
O	-2.007083	-1.147171	0.302065
H	-2.943786	-1.233129	0.096112
H	-1.546939	-0.899354	-0.525116

Vibrational Frequencies

64.0566	145.2833	164.3304
176.4764	177.4713	210.6228
239.0294	248.0227	271.7680
322.2332	368.4362	433.0139
544.7650	585.9570	642.3687
773.9827	844.4747	891.9884
899.5075	1097.3579	1122.5627
1153.5287	1239.9672	1305.4898
1378.4101	1407.1620	1470.1590
1491.8280	1556.0458	1562.5486
1646.0052	1653.2075	3104.2092
3114.0353	3176.7539	3198.0461
3612.2180	3639.9128	3684.6992
3723.7457	3956.2800	3960.2047

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Cartesian Coordinates

C	1.095910	-1.140342	-0.234415
C	1.993141	0.060553	-0.063886
H	1.722849	-2.038385	-0.245808
O	0.169457	-1.205272	0.839814
H	0.583269	-1.066893	-1.197325
H	2.825875	0.003011	-0.770525
O	1.217279	1.246816	-0.328439
H	-0.721002	-1.330495	0.467028
H	2.380928	0.081295	0.956888
H	1.776037	2.023271	-0.193393
O	-2.344384	-0.899738	-0.358740
H	-2.841750	-1.072211	-1.164496
H	-2.240191	0.070784	-0.280163
O	-1.518811	1.671396	0.216001
H	-0.562259	1.502106	0.105584
H	-1.646397	1.800632	1.162925

Vibrational Frequencies

29.8304	63.0533	82.5710
152.6727	163.4306	192.2500
209.9085	238.2428	261.6093
301.5993	332.1212	373.8594
419.0585	513.6823	674.9759
709.6037	891.3216	900.8112
943.2563	1079.6845	1115.5110
1137.5623	1232.7073	1275.7678
1342.9598	1400.3880	1444.8789
1495.7174	1542.2633	1547.5251
1655.7017	1680.0288	3089.8879
3108.6394	3157.0788	3177.5507
3595.8081	3670.2801	3734.9824
3879.0682	3945.3176	3965.6073

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Cartesian Coordinates

C	-1.522976	-0.259354	-0.905751
C	-0.786865	-1.123370	0.104422
H	-2.601457	-0.408096	-0.823652
O	-1.226336	1.138778	-0.703042
H	-1.209216	-0.495350	-1.921491
H	0.280580	-1.147812	-0.111503
O	-1.029119	-0.630703	1.430103
H	-1.726281	1.398539	0.084580
H	-1.170257	-2.143987	0.056659
H	-0.267067	-0.086555	1.674404
O	2.611419	-0.829758	-0.583382
H	3.441862	-1.102922	-0.179998
H	2.355055	-0.001374	-0.144119
O	1.234597	1.389683	0.551583
H	1.565163	2.288185	0.665589
H	0.466184	1.451716	-0.054591

Vibrational Frequencies

30.0855	44.5261	80.4751
115.3161	139.2214	174.6805
188.0762	217.4580	284.0949
292.7827	355.9423	368.4691
433.3338	534.7729	568.2127
643.6995	827.8520	887.8021
914.8724	1055.4569	1078.0965
1127.0310	1216.0278	1289.6048
1398.6933	1408.6232	1426.9254
1465.6281	1542.1840	1561.3136
1656.3718	1674.6349	3132.6121
3141.7923	3210.2291	3223.7847
3585.3215	3744.7302	3849.9430
3852.0171	3942.7902	3968.8372

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Cartesian Coordinates

C	1.839515	-0.746730	0.500180
C	2.247219	0.681168	0.181495
H	1.158086	-0.759038	1.353491
O	1.221365	-1.352304	-0.634916
H	2.726677	-1.331572	0.752571
H	3.039609	0.683718	-0.571335
O	1.127558	1.448480	-0.290457
H	0.263184	-1.225153	-0.521389
H	2.610294	1.189315	1.074782
H	0.932813	1.111336	-1.176723
O	-4.051056	0.156609	-0.006658
H	-4.490830	-0.163233	-0.802950
H	-4.597306	-0.137495	0.731559
O	-1.203200	-0.202067	0.256623
H	-2.155652	-0.040730	0.160957
H	-0.764607	0.660479	0.312252

Vibrational Frequencies

19.6520	39.6056	71.1078
96.6919	118.2558	145.4006
186.4785	190.9937	219.8155
254.1611	299.8680	365.8389
490.3883	531.2152	546.3549
698.6749	759.2049	890.3503
905.1220	1063.7974	1097.2958
1135.1665	1223.7915	1288.6288
1402.1678	1424.5631	1443.8712
1452.5055	1538.4174	1542.8063
1638.5093	1659.8465	3118.1133
3120.8744	3184.0111	3203.4198
3731.4128	3761.4617	3850.5851
3859.8474	3881.2814	4000.8131

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Cartesian Coordinates

C	2.081734	-0.429462	-0.190143
C	0.717096	-1.053545	-0.373809
H	2.683673	-0.574952	-1.086194
O	1.982830	0.985901	0.003535
H	2.593428	-0.896710	0.655197
H	0.813167	-2.137903	-0.483719
O	-0.047642	-0.720717	0.790197
H	1.675070	1.123345	0.909439
H	0.239110	-0.649025	-1.270595
H	-0.964446	-1.024088	0.647621
O	-1.302350	1.721530	-0.031627
H	-0.643371	1.112073	0.347934
H	-0.809432	2.266044	-0.656661
O	-2.667713	-0.705710	-0.197485
H	-3.576363	-0.822689	0.099681
H	-2.524820	0.253906	-0.295949

Vibrational Frequencies

46.8397	63.7998	73.4961
135.7154	175.0106	202.2166
214.1506	223.7944	300.6988
321.5601	338.2089	364.8984
421.2045	542.2810	618.2096
665.5954	887.0072	897.9069
915.1852	1062.3130	1129.7485
1135.0438	1212.8609	1282.0366
1355.3316	1401.8896	1432.5631
1492.5021	1540.4417	1557.5686
1648.0656	1668.8243	3099.0873
3122.2844	3160.5506	3208.5328
3667.8108	3719.2136	3726.9090
3870.7496	3946.5628	3963.3767

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Cartesian Coordinates

C	2.246180	-0.517583	0.412900
C	1.613280	0.849848	0.597939
H	2.524861	-0.947308	1.375307
O	1.326635	-1.443678	-0.186763
H	3.142482	-0.430273	-0.206388
H	2.357710	1.545435	0.991088
O	1.150892	1.365909	-0.647130
H	1.232102	-1.171798	-1.111199
H	0.790395	0.782256	1.314775
H	0.227945	1.070215	-0.746106
O	-3.958291	-0.050294	0.364662
H	-4.630110	-0.269839	-0.291402
H	-4.271713	0.748497	0.804609
O	-1.223335	-0.156784	-0.519993
H	-2.135992	-0.148504	-0.188326
H	-0.761650	-0.893502	-0.093599

Vibrational Frequencies

18.8612	33.3914	74.2274
94.7348	114.4560	153.5136
182.1094	197.7674	219.8513
255.3337	312.5309	376.3828
495.3398	528.7660	546.4353
701.2372	769.3739	891.4733
900.9410	1066.7651	1100.0418
1136.0296	1221.9674	1285.6082
1399.7949	1423.7344	1445.7357
1449.0059	1536.5660	1540.5499
1637.9016	1654.5124	3110.1573
3120.1658	3177.5894	3200.4708
3717.1470	3755.3690	3848.0707
3859.9423	3890.4986	4000.0323

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Cartesian Coordinates

C	0.936957	-0.331272	0.848823
C	2.171269	0.405083	0.369774
H	0.523936	0.139901	1.745372
O	-0.041363	-0.373638	-0.202030
H	1.186836	-1.368210	1.069325
H	2.953848	0.375510	1.127984
O	2.707070	-0.214243	-0.795784
H	-0.498147	0.491180	-0.234915
H	1.920042	1.453894	0.172558
H	1.954687	-0.365293	-1.387417
O	-2.742616	-1.118159	-0.146769
H	-1.774659	-1.239134	-0.135516
H	-3.121008	-1.822625	0.389657
O	-2.019994	1.565927	-0.029781
H	-2.400074	2.215865	-0.630750
H	-2.619600	0.796943	-0.032976

Vibrational Frequencies

27.9672	39.0950	77.2136
125.5773	170.1790	191.6728
205.7803	239.3651	264.5050
344.9241	370.0902	419.4024
461.1672	548.2892	593.8426
693.3334	881.7043	901.9752
918.4218	1075.0888	1123.5667
1130.3950	1224.1279	1273.1990
1387.2228	1421.2524	1448.7300
1462.7086	1540.1610	1551.6810
1648.3280	1670.7754	3087.6262
3116.8536	3189.4597	3208.1506
3631.9354	3694.0375	3719.7433
3834.2241	3960.9967	3965.2330

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Cartesian Coordinates

C	-0.772996	-0.268707	0.952652
C	-1.254419	-0.782686	-0.381636
H	0.122951	-0.804481	1.265789
O	-0.468852	1.140683	0.755712
H	-1.565780	-0.362937	1.696148
H	-1.496529	-1.840975	-0.302124
O	-2.450241	-0.120871	-0.795425
H	-0.452039	1.579643	1.616387
H	-0.460617	-0.669231	-1.124928
H	-2.268587	0.828307	-0.750607
O	2.148569	-1.450125	0.077833
H	2.311396	-0.540551	-0.230682
H	3.014325	-1.862556	0.162821
O	2.006508	1.292131	-0.560183
H	1.951024	1.712107	-1.425460
H	1.120471	1.374484	-0.156933

Vibrational Frequencies

28.3674	45.5630	74.5050
105.8682	171.7282	173.1295
209.9938	218.6382	245.3803
302.6603	344.0859	367.6422
424.0591	462.5052	531.0962
705.6555	781.9005	884.0944
921.6262	1047.6649	1107.6515
1128.2623	1183.1251	1296.1143
1306.2631	1389.7822	1433.4017
1477.4157	1544.0516	1553.4227
1655.2385	1676.0260	3125.0307
3135.5830	3212.5117	3217.4333
3647.9643	3715.7931	3857.3713
3881.2495	3955.2355	3965.5694

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Cartesian Coordinates

C	1.742977	0.588921	0.213027
C	1.140272	-0.709147	0.716769
H	2.691767	0.395273	-0.292433
O	0.837567	1.226612	-0.705027
H	1.910352	1.294633	1.025567
H	0.263087	-0.496984	1.331635
O	0.777034	-1.500210	-0.414924
H	0.671933	0.554815	-1.387673
H	1.871921	-1.249287	1.323348
H	-0.191320	-1.616106	-0.390330
O	-2.004176	-1.222553	-0.183658
H	-2.104602	-0.272336	0.025629
H	-2.644336	-1.694954	0.359032
O	-1.706273	1.492069	0.352848
H	-2.200067	2.261776	0.049317
H	-0.801451	1.577184	-0.016783

Vibrational Frequencies

50.3519	65.8902	110.2087
177.2061	200.3353	211.3107
224.6539	229.5253	268.3316
315.1298	396.2991	464.6374
531.9712	570.9987	721.2613
780.1665	845.7518	904.3139
928.6975	1074.8350	1106.8288
1132.7959	1223.6595	1291.7732
1398.8889	1413.1719	1437.3294
1463.1756	1544.9348	1551.1099
1661.5083	1687.7809	3112.4217
3129.4143	3179.3144	3212.9377
3563.4505	3642.0398	3700.5227
3795.3073	3950.0361	3959.2998

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Cartesian Coordinates

C	0.800504	-0.241440	0.989272
C	1.308350	0.803332	0.025761
H	-0.057172	0.139110	1.539165
O	0.355920	-1.406657	0.271828
H	1.590240	-0.526795	1.688482
H	1.694155	1.665034	0.576656
O	2.359983	0.157723	-0.719220
H	1.056569	-1.601695	-0.370878
H	0.499508	1.127451	-0.628104
H	2.543176	0.674525	-1.513254
O	-2.265152	-1.035630	-0.520387
H	-2.844809	-1.674649	-0.091779
H	-1.351147	-1.300677	-0.287421
O	-1.834750	1.665747	0.119821
H	-2.176130	0.785816	-0.127820
H	-2.535513	2.291065	-0.091577

Vibrational Frequencies

29.0552	51.6485	75.8324
97.5884	159.5900	164.5838
216.1611	251.0101	257.8225
294.4869	335.7762	370.0454
439.1416	526.5017	553.0364
711.4145	818.1355	900.9478
919.0193	1065.7563	1099.7074
1124.9744	1191.9598	1276.6155
1306.4489	1390.2106	1438.0373
1481.7916	1545.7103	1561.1328
1662.0791	1686.8921	3120.9789
3129.7359	3207.0847	3231.1753
3596.9722	3685.8452	3815.6149
3895.3898	3952.9472	3963.2057

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Cartesian Coordinates

C	-0.178606	0.740354	1.278871
C	0.178606	-0.740354	1.278871
H	0.301357	1.211028	2.142432
O	0.178606	1.421910	0.070293
H	-1.256347	0.870278	1.377645
H	-0.301357	-1.211028	2.142432
O	-0.178606	-1.421910	0.070293
H	1.011352	1.051726	-0.279893
H	1.256347	-0.870278	1.377645
H	-1.011352	-1.051726	-0.279893
O	-2.070943	0.351114	-1.070291
H	-2.427894	0.486031	-1.954490
H	-1.323387	0.972268	-0.958939
O	2.070943	-0.351114	-1.070291
H	2.427894	-0.486031	-1.954490
H	1.323387	-0.972268	-0.958939

Vibrational Frequencies

70.5171	155.3579	163.9372
171.7031	183.8253	225.1357
237.9432	245.7851	255.8654
330.0736	408.6062	455.1486
508.5580	560.6608	654.6095
706.3288	864.5015	891.7641
909.3630	1095.1550	1125.0499
1151.8640	1245.7682	1304.3709
1386.9213	1406.8908	1479.0351
1492.9692	1557.2978	1563.9374
1645.1762	1651.8137	3106.0997
3115.6571	3181.3869	3201.0896
3615.6123	3639.3838	3697.3645
3708.3703	3960.4217	3960.7917

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Cartesian Coordinates

C	-0.286375	1.364104	-0.645728
C	0.445006	1.285653	0.685445
H	0.093594	2.212153	-1.218031
O	-0.085261	0.184424	-1.437658
H	-1.354993	1.511807	-0.478479
H	0.195987	2.161516	1.287359
O	0.063640	0.122166	1.435801
H	-0.829380	-0.410035	-1.230564
H	1.523640	1.272362	0.521475
H	0.720004	-0.563791	1.211461
O	1.939234	-1.243495	-0.137755
H	2.160717	-2.143449	-0.400248
H	1.377578	-0.870055	-0.845523
O	-1.977471	-1.194522	0.102466
H	-1.466358	-0.766716	0.818198
H	-2.893706	-1.250921	0.393216

Vibrational Frequencies

62.5378	132.2046	168.1458
178.4925	182.0043	201.6750
227.1804	242.0491	254.3114
327.6048	376.3391	442.4182
548.4836	593.2828	636.0678
762.3612	862.0891	887.5170
910.0363	1076.3206	1104.5932
1134.8334	1248.4905	1304.8336
1425.7592	1443.7697	1449.0591
1461.8543	1538.5796	1542.7460
1642.6183	1658.1142	3125.3227
3131.1073	3188.4913	3203.4486
3623.6198	3646.0728	3714.7684
3733.7790	3958.1840	3961.3408

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Cartesian Coordinates

C	0.746684	-0.150908	0.964619
C	1.294293	0.798315	-0.079134
H	-0.149503	0.262238	1.421625
O	0.372995	-1.393268	0.342782
H	1.493321	-0.347476	1.741034
H	1.624257	1.733097	0.379408
O	2.366070	0.157229	-0.799904
H	1.083950	-1.594107	-0.287501
H	0.529293	1.025299	-0.816196
H	3.174708	0.222157	-0.275060
O	-2.303456	-1.081684	-0.361648
H	-2.572350	-1.558930	-1.153763
H	-1.382581	-1.355168	-0.175381
O	-1.841591	1.661046	0.044005
H	-2.614048	2.210758	0.210893
H	-2.185062	0.771103	-0.159847

Vibrational Frequencies

30.0353	59.6988	74.6402
97.3068	158.5100	171.2891
207.1380	219.0245	249.0153
302.8642	339.2752	386.4070
444.3997	539.0497	575.0246
709.4601	739.7738	888.8487
905.7394	1062.5449	1068.0158
1111.6969	1214.8155	1250.7452
1376.7521	1381.2695	1422.3865
1463.6578	1540.6407	1553.6326
1668.2033	1697.1673	3103.2155
3138.6032	3227.5767	3247.1778
3622.7475	3693.5232	3802.8179
3873.6850	3957.7993	3964.3060

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Cartesian Coordinates

C	1.785191	0.483014	0.048993
C	1.483649	-0.990916	-0.142835
H	1.758658	0.992231	-0.922141
O	0.905424	1.109501	0.970347
H	2.796299	0.582660	0.448046
H	1.514570	-1.506617	0.815577
O	0.163890	-1.224697	-0.661247
H	0.089726	1.326141	0.486315
H	2.229927	-1.436758	-0.808904
H	-0.020793	-0.569232	-1.351814
O	-1.359230	1.323499	-0.779233
H	-1.894026	2.066176	-1.081143
H	-1.954126	0.713581	-0.295820
O	-2.268065	-0.841497	0.634657
H	-1.396929	-1.190685	0.358604
H	-2.272491	-0.864539	1.598150

Vibrational Frequencies

40.5748	77.8213	102.1090
152.1616	199.2556	228.3878
236.3401	278.8319	289.9341
327.7182	394.9481	423.4814
458.6994	535.7559	638.2105
791.9835	824.5783	888.6244
907.6260	1079.1873	1114.7911
1146.8069	1214.4693	1307.6478
1377.3934	1433.2390	1452.6568
1465.8606	1538.4900	1545.2801
1656.0691	1687.9195	3082.5282
3104.5614	3173.6240	3207.4545
3595.3834	3659.8073	3747.3452
3823.8255	3950.9967	3951.7437

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Cartesian Coordinates

C	1.221027	-1.110161	-0.485799
C	1.491797	-0.306478	0.774113
H	1.319176	-2.179452	-0.266917
O	-0.069060	-0.840681	-1.055426
H	1.942875	-0.840958	-1.254340
H	2.433099	-0.646469	1.209760
O	1.642464	1.083673	0.542784
H	-0.747210	-1.078281	-0.402440
H	0.697092	-0.505614	1.506971
H	0.788287	1.455149	0.255674
O	-0.930223	1.817289	-0.580967
H	-0.682252	1.054279	-1.131994
H	-1.670901	1.479633	-0.060572
O	-2.457517	-0.628680	0.659497
H	-3.286533	-0.940617	0.274512
H	-2.555893	-0.750641	1.612368

Vibrational Frequencies

31.6899	47.9536	85.0741
126.9640	152.1283	174.5933
193.3670	236.7590	264.3371
290.5470	319.5425	355.7110
426.4968	512.1186	557.3532
695.8902	797.4418	876.4277
915.5410	1084.5395	1108.8749
1147.3862	1221.5395	1298.0509
1409.3623	1425.5884	1442.1053
1462.8150	1535.7772	1537.6569
1644.9133	1697.4091	3055.3505
3094.9465	3169.9936	3215.1015
3698.4959	3755.2302	3794.9659
3842.8379	3921.8159	3978.8844

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Cartesian Coordinates

C	1.339749	-0.840236	-0.616490
C	1.567863	-0.129811	0.699579
H	1.797484	-1.828414	-0.564820
O	-0.040618	-1.049439	-0.907447
H	1.822465	-0.276793	-1.419540
H	2.634064	-0.162138	0.944136
O	1.138662	1.237248	0.555798
H	-0.434247	-0.201450	-1.201595
H	0.999079	-0.624877	1.490284
H	1.254231	1.685155	1.404233
O	-2.081581	-0.718861	0.984815
H	-2.781896	-1.368697	1.108575
H	-1.400740	-1.145885	0.431640
O	-1.363630	1.412814	-0.893187
H	-1.957390	0.994540	-0.248648
H	-0.601393	1.694746	-0.362636

Vibrational Frequencies

46.5904	60.3167	128.6410
152.9870	179.3267	197.3910
227.0294	237.4026	308.0370
340.1444	356.1433	419.9945
505.1922	547.6428	592.3178
686.3430	866.8349	905.3323
914.9785	1084.3208	1127.1398
1135.4290	1226.6830	1278.5228
1338.0553	1429.0516	1480.0408
1488.0461	1533.4327	1549.3740
1644.7009	1690.1013	3100.1880
3120.5305	3168.9928	3197.5542
3596.8002	3685.0828	3765.7008
3869.3750	3876.7960	3957.3816

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Cartesian Coordinates

C	-1.989968	-0.428827	-0.086330
C	-0.681887	-1.177869	-0.178263
H	-2.398900	-0.529578	0.921307
O	-1.722247	0.954004	-0.387522
H	-2.699864	-0.838703	-0.810975
H	-0.219763	-0.965611	-1.148872
O	0.210364	-0.867186	0.890943
H	-2.476878	1.485685	-0.104188
H	-0.874263	-2.248707	-0.114296
H	0.342718	0.105408	0.906659
O	2.625650	-0.458143	-0.519612
H	2.007002	-0.903614	0.088140
H	3.503115	-0.801732	-0.320048
O	0.994945	1.757235	0.342305
H	1.727089	1.380624	-0.172663
H	0.251178	1.869119	-0.266425

Vibrational Frequencies

55.3457	69.9951	113.4239
143.0379	155.3601	183.6666
199.4417	232.3271	254.2374
349.5133	369.5419	414.9762
472.8926	541.6128	569.0578
620.4238	893.9711	914.1213
933.7187	1085.6930	1114.2497
1134.1049	1227.0791	1287.7309
1327.1467	1424.2848	1464.2568
1493.0595	1540.6427	1550.6411
1641.9311	1659.3276	3099.0793
3103.3764	3173.5792	3194.6734
3575.0472	3699.2802	3770.4945
3885.4894	3915.3458	3961.0034

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Cartesian Coordinates

C	1.298399	-1.036242	0.364911
C	1.329234	-0.110688	-0.831686
H	2.125584	-0.795825	1.034352
O	0.039331	-0.855519	1.064916
H	1.377395	-2.074638	0.032336
H	0.442255	-0.277958	-1.448297
O	1.459751	1.255825	-0.462467
H	0.055431	-1.397652	1.865475
H	2.209680	-0.361683	-1.424910
H	0.574135	1.598325	-0.258986
O	-2.273039	-0.956386	-0.870589
H	-1.580328	-1.144316	-0.222272
H	-2.385788	0.000385	-0.796805
O	-1.240445	1.579445	0.501401
H	-0.919601	0.861745	1.073799
H	-1.549340	2.286279	1.079862

Vibrational Frequencies

45.4087	65.4314	86.3061
123.1113	159.1363	186.7584
221.2297	257.5152	283.2616
335.7776	349.4776	386.6007
429.6608	464.1954	515.3911
568.9240	743.5230	876.7374
914.4589	1063.9960	1118.3148
1134.3681	1213.1156	1282.9511
1335.1872	1433.8309	1453.9158
1476.8212	1534.8346	1543.8813
1625.0586	1685.6431	3114.1312
3123.0019	3186.4891	3195.6105
3737.8806	3785.6280	3823.5945
3868.8745	3942.4799	3957.6496

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Cartesian Coordinates

C	1.856808	0.167936	0.294049
C	0.835199	-0.875820	0.717639
H	2.746058	-0.310824	-0.114699
O	1.328047	0.964209	-0.766746
H	2.148581	0.776555	1.154354
H	0.035594	-0.405892	1.295135
O	0.268900	-1.497856	-0.452209
H	0.535728	1.430098	-0.432695
H	1.295599	-1.657074	1.322447
H	0.459461	-0.875214	-1.177480
O	-2.347211	-0.738708	-0.010654
H	-3.060268	-1.141426	-0.517609
H	-1.527895	-1.229142	-0.234238
O	-1.165299	1.780893	0.272023
H	-1.764274	1.017585	0.150153
H	-1.696132	2.574336	0.145183

Vibrational Frequencies

62.2061	84.5713	117.4464
169.7661	180.1797	210.5965
220.2719	225.8037	228.4885
335.7454	413.0045	512.4438
564.3922	567.7399	647.1680
777.1251	880.8837	902.0952
924.0555	1084.1756	1118.7916
1130.5051	1244.3627	1263.2790
1370.0636	1413.0298	1461.8475
1482.7109	1549.9341	1569.3988
1669.3284	1690.9934	3117.5284
3129.2651	3190.9058	3206.7190
3571.8672	3643.1258	3676.8110
3737.7898	3955.6919	3960.6374

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Cartesian Coordinates

C	-2.220675	0.294506	0.451342
C	-0.975504	-0.497311	0.777993
H	-2.010253	1.363778	0.565573
O	-2.676211	0.006991	-0.866861
H	-3.030540	0.026343	1.128653
H	-1.181024	-1.565893	0.687608
O	0.015028	-0.105485	-0.184426
H	-1.898298	0.085832	-1.438782
H	-0.634912	-0.280110	1.795283
H	0.732605	-0.769558	-0.203582
O	2.317798	1.497003	-0.075779
H	2.443696	2.253637	0.506444
H	1.366602	1.281732	-0.061710
O	2.528160	-1.283089	-0.071167
H	3.068614	-1.741554	-0.723677
H	2.842385	-0.360741	-0.045955

Vibrational Frequencies

30.0474	34.4839	76.1117
128.2635	177.0369	197.4691
201.9812	223.8567	265.6316
346.4586	362.9401	417.6793
464.1629	543.7509	590.9365
692.3743	877.8533	899.4631
921.5335	1077.2054	1127.7717
1145.6708	1217.4635	1284.1872
1361.8159	1391.4281	1442.7231
1489.7834	1547.0055	1553.3387
1649.5017	1670.8114	3094.0536
3101.3751	3172.7773	3200.3188
3639.9686	3699.6023	3725.7631
3839.4312	3961.7459	3964.8572

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Cartesian Coordinates

C	-2.049044	-0.341553	-0.062260
C	-0.804444	-1.162661	-0.278646
H	-2.423123	-0.518946	0.948947
O	-1.696996	1.040503	-0.235510
H	-2.814010	-0.634619	-0.787377
H	-0.357626	-0.897172	-1.241233
O	0.092973	-0.885835	0.793448
H	-2.417089	1.586102	0.105052
H	-1.075186	-2.223366	-0.299422
H	0.995546	-1.122132	0.508284
O	1.231386	1.706531	0.196927
H	0.766538	2.263563	-0.438296
H	0.534328	1.115665	0.537941
O	2.621258	-0.628730	-0.371622
H	2.390357	0.317393	-0.281402
H	3.532221	-0.720963	-0.072998

Vibrational Frequencies

47.8912	65.6186	82.6071
118.4761	183.9181	202.3800
225.6801	230.9341	248.9194
277.2938	332.1787	351.1455
400.5415	525.3220	631.0423
709.7441	904.5057	913.7912
931.7556	1090.0040	1104.4189
1136.8737	1236.8707	1281.1898
1327.3195	1369.1872	1449.1620
1510.7639	1548.7624	1553.4014
1652.3278	1666.9245	3091.9095
3104.6163	3152.8600	3170.8793
3630.5602	3706.3295	3734.8941
3884.9069	3948.0372	3959.6367

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Cartesian Coordinates

C	-1.742221	0.344159	0.577212
C	-0.623631	-0.665707	0.652595
H	-1.331383	1.333156	0.366994
O	-2.588662	-0.103666	-0.495636
H	-2.290004	0.368888	1.523191
H	-1.022637	-1.653071	0.896245
O	0.076461	-0.719066	-0.603737
H	-3.187722	0.610411	-0.746293
H	0.110587	-0.374695	1.400531
H	-0.597194	-0.876241	-1.283961
O	2.807874	-0.767515	0.124378
H	3.498295	-1.367690	-0.176163
H	1.989179	-1.045584	-0.317261
O	1.428079	1.879448	-0.104409
H	2.252670	1.456776	0.173077
H	0.983310	1.163735	-0.579970

Vibrational Frequencies

22.9033	36.6031	72.8649
92.5168	125.6068	136.5750
158.7832	235.6460	270.7420
292.4090	344.0718	363.5293
386.7616	502.1601	537.3308
550.7636	602.5503	898.3715
916.5149	1062.9749	1105.2911
1128.2500	1181.8489	1278.5170
1306.4657	1390.3029	1439.5703
1482.1175	1542.9605	1562.3338
1637.9707	1690.6252	3113.1488
3132.6637	3186.4744	3230.3677
3768.2170	3817.3426	3827.2717
3892.4835	3927.4942	3972.7447

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Cartesian Coordinates

C	1.957061	-0.034686	0.252625
C	0.776293	-0.822796	0.771045
H	2.696301	-0.702439	-0.195647
O	1.415009	0.845786	-0.751902
H	2.416974	0.535688	1.062511
H	0.084793	-0.147487	1.278181
O	0.109686	-1.489466	-0.312781
H	2.135907	1.275477	-1.229993
H	1.109051	-1.594198	1.463833
H	0.185186	-0.896128	-1.077898
O	-1.191199	1.950109	0.408024
H	-0.397474	1.828628	-0.129451
H	-1.784111	1.226552	0.149312
O	-2.551809	-0.580365	-0.273081
H	-3.304270	-1.002534	0.154938
H	-1.795973	-1.187179	-0.179885

Vibrational Frequencies

53.1619	63.2808	95.0836
118.8000	164.0061	183.2935
192.1908	202.9089	285.8275
329.5640	357.5983	460.8073
487.7456	528.1229	549.0189
632.6308	698.4921	896.6929
914.8196	1069.5382	1105.6507
1138.4226	1194.3966	1279.6604
1304.2776	1388.2514	1443.0209
1487.6796	1554.4740	1559.0059
1644.2034	1690.1053	3115.6473
3140.9927	3182.5724	3216.0763
3710.9379	3774.7772	3803.1815
3885.5749	3918.5443	3964.9261

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Cartesian Coordinates

C	-1.398656	-1.184486	-0.325901
C	0.099928	-1.178681	-0.110696
H	-1.743215	-2.219628	-0.306031
O	-2.113236	-0.500760	0.694430
H	-1.620809	-0.768479	-1.314154
H	0.569075	-1.880698	-0.808016
O	0.605695	0.145749	-0.346039
H	-2.052374	0.453266	0.511432
H	0.316911	-1.490435	0.913908
H	1.556606	0.157098	-0.143610
O	-1.330339	2.107075	-0.181458
H	-0.487768	1.618887	-0.261975
H	-1.160953	2.856026	0.399724
O	3.406912	0.097011	0.212634
H	4.055391	0.322747	-0.464532
H	3.807249	0.337631	1.056296

Vibrational Frequencies

21.9840	42.7357	70.4463
96.8653	131.8070	160.9438
171.8561	206.1053	216.2638
245.0234	275.0498	355.8527
401.9759	518.2320	558.2243
716.7278	782.0498	886.1541
920.6748	1088.4563	1132.4993
1140.1836	1246.1266	1294.0413
1361.0204	1429.5741	1471.9630
1488.6489	1531.5724	1546.6120
1643.9830	1664.8752	3092.5555
3103.0117	3162.4857	3181.9997
3649.4183	3740.7117	3760.5995
3859.7509	3961.0505	3999.9127

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Cartesian Coordinates

C	1.369915	-0.914965	0.468515
C	1.330226	-0.105434	-0.813179
H	2.130110	-0.502200	1.143705
O	0.107280	-1.000346	1.121245
H	1.653490	-1.941308	0.233758
H	0.491215	-0.417459	-1.430892
O	1.111363	1.301212	-0.560043
H	-0.239658	-0.106607	1.280370
H	2.260757	-0.238184	-1.371670
H	1.901115	1.663320	-0.135984
O	-1.394931	1.449645	0.599002
H	-0.608152	1.719576	0.090538
H	-1.825190	2.253132	0.911819
O	-2.098090	-1.082161	-0.895073
H	-1.525682	-1.467710	-0.216100
H	-2.243831	-0.186960	-0.558607

Vibrational Frequencies

53.1566	72.2826	84.3193
121.5938	167.4575	183.2214
239.0628	241.6354	294.4344
309.1641	348.6244	381.1332
439.3280	523.6277	551.0119
660.7490	692.0886	872.8032
908.9276	1067.8118	1083.2654
1138.6401	1214.0277	1273.5303
1389.0299	1405.4289	1434.1867
1462.0269	1538.6686	1540.8239
1646.2364	1692.7782	3077.2787
3122.7716	3187.4966	3231.2116
3698.5235	3782.8470	3814.1169
3868.1674	3921.5117	3958.8920

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Cartesian Coordinates

C	1.102383	-0.737736	0.707069
C	1.748439	0.552059	0.236996
H	0.214941	-0.516512	1.303140
O	0.747514	-1.497496	-0.450530
H	1.805487	-1.305766	1.321910
H	2.706893	0.343246	-0.243892
O	0.883931	1.219085	-0.699647
H	-0.217608	-1.630206	-0.417311
H	1.908204	1.244039	1.062663
H	0.708262	0.547765	-1.380558
O	-1.669862	1.528284	0.310988
H	-0.760007	1.601707	-0.048536
H	-2.118704	2.356367	0.110131
O	-2.013768	-1.216372	-0.033756
H	-2.813371	-1.544055	-0.458255
H	-2.121551	-0.250528	0.069871

Vibrational Frequencies

53.3017	60.4700	103.4996
162.3835	186.3780	202.3932
217.6758	228.8345	234.5582
317.0828	404.8117	512.5867
539.3190	562.3286	638.5625
706.0157	846.1937	902.4872
929.4515	1073.9619	1107.4414
1134.5018	1226.1590	1292.6180
1398.5577	1415.1280	1441.8345
1470.7183	1545.8784	1554.5318
1666.0022	1679.9297	3114.1522
3128.5237	3182.8436	3213.3004
3566.1066	3657.9972	3716.9107
3791.3885	3956.1588	3964.3806

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Cartesian Coordinates

C	0.119556	-0.608694	0.687226
C	-0.087380	0.882092	0.550649
H	-0.840033	-1.112639	0.797983
O	0.766067	-1.039876	-0.535705
H	0.762449	-0.824191	1.543750
H	0.874169	1.387781	0.447141
O	-0.930409	1.178446	-0.574435
H	0.548966	-1.967971	-0.691327
H	-0.603045	1.269159	1.427755
H	-0.482010	0.812244	-1.351353
O	3.238801	0.211888	0.035537
H	2.557370	-0.359195	-0.355518
H	4.040090	0.068976	-0.478560
O	-3.134620	-0.477678	0.020301
H	-4.029633	-0.130644	-0.054069
H	-2.540099	0.233851	-0.278639

Vibrational Frequencies

20.6080	26.8904	66.1380
97.4038	108.6931	149.5668
167.4260	202.7700	210.1888
287.8883	337.7608	372.5272
405.0739	489.0251	540.6331
593.6361	714.1687	894.6460
914.5326	1056.1395	1096.9103
1122.9528	1189.8520	1298.2436
1314.4863	1402.6859	1434.9059
1480.0015	1547.4045	1555.1915
1649.2662	1652.5215	3127.8140
3145.7861	3208.9714	3225.1399
3698.3184	3752.4232	3844.1831
3888.2996	3963.4540	3971.2460

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Cartesian Coordinates

C	1.853771	-0.612350	0.614960
C	1.627058	0.862110	0.379099
H	0.888590	-1.107353	0.748314
O	2.594659	-1.198083	-0.455201
H	2.448662	-0.756050	1.515832
H	2.583936	1.368559	0.239879
O	0.840154	0.957171	-0.830893
H	2.107713	-0.992723	-1.265873
H	1.082877	1.305492	1.216049
H	0.908730	1.855172	-1.179757
O	-4.177879	-0.442605	-0.313252
H	-4.905784	0.085030	0.035227
H	-4.416366	-1.360885	-0.141137
O	-1.538279	0.366240	0.678972
H	-0.943820	0.538106	-0.066283
H	-2.388763	0.104313	0.296381

Vibrational Frequencies

13.6820	28.5199	39.6233
72.4457	79.4026	140.0538
162.7262	176.2282	209.4750
239.7277	283.8354	337.7500
435.5832	513.4585	532.2857
622.3779	669.3644	890.9607
916.8139	1059.7012	1103.7668
1129.5093	1182.5821	1288.3385
1306.8021	1396.2457	1434.2490
1476.7007	1546.9789	1550.9394
1636.3327	1669.6382	3119.0387
3129.3661	3189.0646	3210.7803
3767.1006	3854.8050	3859.6874
3884.3500	3894.7360	4001.7074

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Cartesian Coordinates

C	-0.713081	-0.993432	0.590837
C	-1.275572	-0.183615	-0.571863
H	-1.512354	-1.466489	1.163577
O	0.241965	-1.983824	0.145315
H	-0.153641	-0.339309	1.255621
H	-2.018121	-0.764701	-1.121817
O	-1.932362	0.982219	-0.098075
H	-0.204744	-2.613159	-0.436860
H	-0.460771	0.066452	-1.257505
H	-1.217986	1.596691	0.147735
O	2.286355	-0.147465	-0.335808
H	3.119508	-0.372758	0.092966
H	1.716635	-0.937070	-0.250878
O	0.690750	2.095227	0.320623
H	1.341172	1.404970	0.085363
H	1.028549	2.918414	-0.048486

Vibrational Frequencies

47.8139	80.3712	145.9414
150.7117	182.7150	202.8702
207.3222	228.4322	244.6066
290.0250	355.9469	412.5151
452.3490	483.0287	665.9214
729.1174	778.4034	819.3047
1026.6424	1076.7559	1111.4778
1116.5073	1171.3824	1327.2106
1350.7621	1398.3093	1458.8671
1466.1707	1552.8123	1562.8770
1669.2181	1688.3708	3109.7423
3145.3677	3176.5973	3232.8644
3632.6892	3676.7124	3747.5545
3869.9290	3950.5922	3955.9411

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Cartesian Coordinates

C	-1.323113	0.788475	-0.053969
C	-0.746787	-0.173830	0.961632
H	-0.564106	1.055211	-0.783652
O	-2.378136	0.139819	-0.790953
H	-1.677122	1.700360	0.432362
H	-1.486773	-0.415548	1.731722
O	-0.335508	-1.385465	0.304234
H	-3.185340	0.161029	-0.260212
H	0.136692	0.252770	1.431677
H	-1.033014	-1.586725	-0.341044
O	1.832349	1.663837	0.112215
H	2.465080	2.309825	-0.218256
H	2.185155	0.789602	-0.138945
O	2.295172	-1.040252	-0.497725
H	1.384796	-1.312901	-0.262472
H	2.883006	-1.665004	-0.059330

Vibrational Frequencies

36.8412	60.2807	77.6531
96.1359	160.1936	165.0029
215.1898	246.3680	253.5951
306.3450	341.2603	371.6619
433.7182	539.7173	567.2924
719.2957	809.1911	893.4931
908.9027	1064.0653	1069.1611
1113.4141	1215.9110	1251.1703
1376.5691	1381.2996	1421.0448
1463.6916	1542.6810	1553.8977
1660.0911	1684.0922	3102.3790
3136.6186	3223.8216	3248.5699
3611.4662	3689.8445	3801.6628
3872.3304	3953.7706	3963.0681

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Cartesian Coordinates

C	-1.505909	-0.149733	-0.739309
C	-1.346411	-0.883008	0.580071
H	-2.516679	-0.317766	-1.114349
O	-1.364211	1.261535	-0.608958
H	-0.797938	-0.550809	-1.472569
H	-1.631418	-1.932973	0.457070
O	-0.011062	-0.797976	1.104960
H	-0.432463	1.466074	-0.432996
H	-1.988045	-0.429514	1.333317
H	0.594256	-1.238847	0.480777
O	2.006125	-0.950606	-0.854419
H	2.192731	-0.032332	-0.594739
H	2.848058	-1.346076	-1.104894
O	1.400918	1.439434	0.514562
H	1.682947	2.162494	1.086088
H	0.908316	0.797096	1.068572

Vibrational Frequencies

51.7268	89.9265	127.8500
163.8970	174.0082	190.7553
208.4589	253.5846	309.0032
339.7542	384.6429	432.5975
456.0905	521.6339	585.6232
754.1415	849.8857	878.8877
920.3863	1082.5005	1110.5067
1138.2770	1223.9846	1296.4384
1412.8061	1429.4981	1441.3808
1460.9422	1535.6777	1539.1939
1630.9030	1653.0825	3098.6013
3107.9555	3181.3359	3213.3054
3583.6824	3724.8093	3760.6019
3806.2443	3949.2132	3967.5193

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Cartesian Coordinates

C	1.919064	-0.043235	0.359904
C	0.719558	-0.907001	0.673319
H	2.717793	-0.642088	-0.083427
O	1.444894	0.928812	-0.592262
H	2.282118	0.444358	1.267147
H	-0.036802	-0.311169	1.188618
O	0.174025	-1.458578	-0.535935
H	2.186576	1.452362	-0.922131
H	1.006384	-1.746075	1.304860
H	0.292419	-0.776759	-1.217028
O	-2.472835	-0.685747	0.019387
H	-3.250542	-1.010091	-0.447181
H	-1.722868	-1.237742	-0.265389
O	-1.283216	2.028055	0.228893
H	-1.800621	1.212437	0.138510
H	-0.409135	1.815844	-0.123979

Vibrational Frequencies

22.2263	73.0029	86.5961
128.1791	162.3102	186.9111
196.4730	208.2986	288.6208
349.7837	379.5337	450.5685
465.4072	492.5650	550.1803
605.1533	750.0363	895.1589
914.5014	1068.6964	1107.0936
1139.5619	1190.0573	1279.2457
1301.2342	1387.1696	1442.9764
1486.8444	1554.9715	1559.9690
1646.5264	1695.3926	3116.7280
3139.2114	3183.8645	3217.1456
3710.3833	3779.4012	3806.0967
3885.4454	3919.0154	3963.8370

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Cartesian Coordinates

C	-0.765910	-0.982460	-0.580877
C	-1.271735	-0.159269	0.593692
H	-0.253005	-0.330055	-1.289812
O	0.161239	-1.964180	-0.053400
H	-1.593989	-1.478057	-1.088723
H	-0.431511	0.071008	1.254304
O	-1.909414	1.023935	0.134599
H	0.242831	-2.688894	-0.687011
H	-2.007374	-0.724310	1.164140
H	-1.189933	1.635451	-0.099377
O	2.306873	-0.202460	0.231495
H	2.844725	-0.324231	1.021779
H	1.675409	-0.949544	0.212373
O	0.737413	2.082675	-0.268536
H	1.175238	2.738855	-0.820740
H	1.394591	1.380398	-0.097088

Vibrational Frequencies

46.0779	81.1523	128.8438
141.2258	161.7539	182.9438
207.9981	236.9817	250.4120
303.1522	330.3269	438.7655
458.4709	483.1087	614.0447
738.4548	808.6515	833.6413
1031.0887	1056.1278	1106.7693
1129.2077	1215.2662	1278.5341
1335.9468	1391.7097	1459.5286
1475.7785	1554.8371	1568.6236
1669.8680	1687.6886	3120.6081
3131.2472	3189.6935	3212.5819
3615.2771	3670.2808	3765.5993
3881.7745	3951.0800	3962.1304

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Cartesian Coordinates

C	-0.873679	-0.871393	0.719850
C	-1.868994	0.187721	0.272585
H	-1.361592	-1.646963	1.310737
O	-0.281178	-1.498554	-0.432811
H	-0.084698	-0.411407	1.320198
H	-2.180037	0.792949	1.128796
O	-1.297346	0.984146	-0.764128
H	-0.450961	-0.881480	-1.168002
H	-2.751199	-0.277279	-0.166470
H	-0.501067	1.425504	-0.405083
O	1.196522	1.762321	0.320468
H	1.767667	0.978821	0.187695
H	1.711562	2.523659	0.031111
O	2.358732	-0.731623	-0.156063
H	2.964870	-1.293706	0.338173
H	1.527648	-1.238392	-0.271484

Vibrational Frequencies

64.3846	87.4501	115.6005
175.6234	206.0048	212.1706
220.3666	238.0725	264.4387
332.9889	391.6429	455.2125
563.8550	625.9351	718.8515
771.7767	883.2380	900.5934
914.0282	1085.2512	1121.3615
1133.7277	1245.2455	1262.5135
1366.6526	1413.9564	1462.5343
1484.9319	1550.6364	1568.1228
1662.1605	1690.7217	3114.9918
3124.5051	3187.4663	3204.2189
3575.2954	3632.0897	3664.7706
3738.9357	3951.2801	3956.8270

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Cartesian Coordinates

C	1.081967	-0.264655	0.956118
C	1.382392	0.065677	-0.494239
H	1.501135	0.507789	1.604309
O	-0.327291	-0.402202	1.174084
H	1.531150	-1.219228	1.222120
H	0.900036	1.008698	-0.766151
O	2.808124	0.161838	-0.595573
H	-0.748049	0.466730	1.036051
H	0.990395	-0.725161	-1.139419
H	3.037624	0.391734	-1.504266
O	-2.168369	-1.172283	-0.752953
H	-1.496954	-1.232826	-0.044623
H	-2.769898	-1.914407	-0.629891
O	-1.911592	1.537407	-0.090220
H	-2.626772	2.161851	0.071731
H	-2.311793	0.750609	-0.503848

Vibrational Frequencies

38.9673	49.2496	71.2487
132.4071	170.1944	189.5291
206.0617	214.0564	220.8640
248.8229	305.4180	367.0028
462.0489	482.7117	569.1055
699.2030	821.6635	856.3869
1033.5568	1079.4211	1103.8785
1149.9191	1232.3674	1249.6231
1339.9439	1386.8678	1451.5329
1491.9749	1560.6200	1577.7894
1643.6139	1668.1356	3102.6564
3135.1379	3161.9319	3222.5280
3633.0993	3705.7860	3729.5539
3890.0773	3957.6747	3963.7530

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Cartesian Coordinates

C	-2.052230	0.215635	0.400652
C	-0.898157	-0.541775	-0.226841
H	-1.794651	1.276290	0.486463
O	-3.178453	0.028445	-0.462813
H	-2.242480	-0.179645	1.401500
H	-0.726888	-0.178437	-1.243178
O	0.281313	-0.416832	0.572776
H	-3.952753	0.436441	-0.056356
H	-1.135147	-1.602728	-0.273378
H	0.641512	0.483338	0.457982
O	2.110344	1.621484	-0.017588
H	2.269743	2.261266	-0.719547
H	2.687561	0.856161	-0.197804
O	2.861060	-1.056839	-0.249446
H	3.415035	-1.639085	0.281434
H	1.946276	-1.166817	0.076587

Vibrational Frequencies

24.0305	43.4236	66.4504
130.3274	159.6356	183.8433
202.7995	208.5951	227.3223
255.1522	306.4496	379.7881
408.4283	498.7174	618.2219
694.5947	834.4751	871.9380
1039.9180	1081.6721	1106.8135
1154.8383	1234.1318	1248.3502
1337.7915	1390.7968	1465.4407
1489.1521	1558.4314	1574.4388
1646.0566	1665.0726	3094.0118
3127.3565	3158.0839	3219.6686
3636.7420	3695.2248	3714.1925
3889.5867	3959.1530	3963.5912

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Cartesian Coordinates

C	-0.865040	-0.550085	-0.182708
C	-2.034156	0.232627	0.382297
H	-0.652978	-0.217350	-1.201277
O	0.287485	-0.410435	0.655071
H	-1.109464	-1.610249	-0.204836
H	-1.781888	1.297375	0.417790
O	-3.142624	-0.004560	-0.491634
H	0.652155	0.486782	0.531747
H	-2.243282	-0.112629	1.398047
H	-3.910288	0.474811	-0.156899
O	2.014627	1.616663	-0.165292
H	2.520573	2.364474	0.169432
H	2.642436	0.880933	-0.286184
O	2.832569	-1.052534	-0.267118
H	3.402034	-1.693536	0.171115
H	1.939425	-1.158933	0.115315

Vibrational Frequencies

28.3115	44.9922	61.7609
120.5785	156.1349	175.7691
181.2594	199.2503	223.2779
232.3592	306.6330	367.0034
462.4386	495.6004	561.5960
703.6335	835.7858	868.2908
1039.4901	1081.8044	1105.1786
1151.1060	1234.5071	1246.1560
1338.1459	1390.6458	1450.9195
1489.3833	1558.3135	1574.2379
1644.4295	1669.4617	3093.4110
3132.7103	3156.0015	3220.4328
3637.0028	3695.4022	3724.9914
3889.6480	3962.1914	3966.8847

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Cartesian Coordinates

C	1.080697	-0.184958	0.968833
C	1.388918	-0.025776	-0.513705
H	1.480625	0.665835	1.530442
O	-0.325493	-0.317320	1.203522
H	1.548129	-1.091018	1.348955
H	0.866312	0.846725	-0.915790
O	2.800414	0.058804	-0.739088
H	-0.756903	0.529610	0.982538
H	1.051926	-0.904522	-1.059691
H	3.107875	0.918152	-0.423616
O	-2.189265	-1.203963	-0.664111
H	-2.789573	-1.944585	-0.527270
H	-1.518488	-1.247560	0.044512
O	-1.897277	1.536611	-0.188685
H	-2.610539	2.168443	-0.047947
H	-2.304084	0.730265	-0.556004

Vibrational Frequencies

36.8947	49.2681	68.9045
145.5266	171.3109	194.7424
210.4985	216.4035	241.2835
262.6626	304.8526	364.8651
456.0443	478.7645	563.9684
694.7959	808.0528	847.4431
1052.6737	1078.0424	1096.1714
1115.4088	1189.6022	1329.3259
1365.8391	1396.3221	1451.2230
1464.7208	1552.0491	1564.8710
1642.3072	1668.1030	3101.6638
3120.9251	3206.5949	3225.1743
3649.7368	3702.3362	3724.3966
3878.4416	3960.1797	3962.6916

199

Cartesian Coordinates

C	1.999185	0.211009	0.386043
C	0.824091	-0.610233	-0.121058
H	2.295573	-0.138489	1.372483
O	3.148320	0.051355	-0.450270
H	1.710956	1.264454	0.465637
H	1.094192	-1.664120	-0.144288
O	-0.302626	-0.491041	0.753512
H	2.957935	0.452232	-1.308333
H	0.555518	-0.297918	-1.136373
H	-0.645861	0.419908	0.676201
O	-2.800282	-0.979313	-0.371370
H	-3.437809	-1.616176	-0.031861
H	-1.955375	-1.148534	0.089553
O	-1.873336	1.640669	-0.115486
H	-2.363234	2.405455	0.205013
H	-2.528161	0.945168	-0.309034

Vibrational Frequencies

27.2988	47.4952	62.9800
141.0222	162.6579	189.6182
195.9811	224.6632	238.0239
286.4008	321.2144	369.3047
463.4343	491.0933	562.8522
692.6471	820.0492	875.7672
1052.5282	1082.2340	1104.7495
1119.9394	1191.1862	1327.7347
1365.2285	1398.6830	1450.9713
1468.0912	1551.0686	1562.9934
1643.1462	1666.6578	3097.0590
3103.2520	3206.7972	3225.1115
3638.4993	3693.6718	3725.5666
3873.5945	3961.9819	3964.7383

201

Cartesian Coordinates

C 2.036764 0.263988 0.372076
 C 0.882009 -0.550801 -0.190927
 H 2.231272 -0.037885 1.404489
 O 3.206375 0.145891 -0.443409
 H 1.783488 1.323375 0.368367
 H 1.135231 -1.611714 -0.195750
 O -0.283165 -0.423274 0.628508
 H 3.552655 -0.750930 -0.350775
 H 0.680415 -0.241175 -1.219777
 H -0.646627 0.475386 0.507242
 O -2.840901 -1.058647 -0.285535
 H -1.943921 -1.166492 0.086607
 H -3.421929 -1.634582 0.222885
 O -2.082246 1.613630 -0.020973
 H -2.218314 2.281236 -0.701546
 H -2.665407 0.862851 -0.237369

Vibrational Frequencies

26.0438 44.2333 69.2299
 142.6582 160.8266 194.6050
 203.5530 225.5557 250.6368
 282.2393 316.0523 380.3618
 405.2264 494.2277 620.1136
 691.1899 817.4147 872.3502
 1053.2140 1085.4600 1101.6843
 1122.7186 1190.3346 1341.4889
 1356.2463 1394.0070 1459.8477
 1472.9750 1551.1963 1563.4947
 1644.2912 1662.5442 3116.3611
 3124.4478 3183.4319 3211.5392
 3638.6365 3691.8905 3717.2288
 3877.1815 3959.0782 3965.2055

202

Cartesian Coordinates

C 1.997881 0.337051 0.279100
 C 0.891884 -0.638973 -0.052260
 H 2.208863 0.296698 1.350663
 O 3.133713 -0.062667 -0.493952
 H 1.679530 1.350808 0.019817
 H 1.202963 -1.650112 0.217742
 O -0.254862 -0.240940 0.707206
 H 3.872610 0.520392 -0.281896
 H 0.683427 -0.606805 -1.124634
 H -0.982554 -0.864813 0.523467
 O -2.777542 -1.140358 -0.123622
 H -3.168747 -1.631408 -0.853786
 H -2.903317 -0.193600 -0.318911
 O -2.127823 1.576073 -0.256483
 H -2.397102 2.326265 0.284366
 H -1.322144 1.207247 0.156943

Vibrational Frequencies

23.4235 36.1764 59.5595
 107.4432 161.7740 181.9282
 196.4341 212.0887 223.4064
 255.2459 316.4451 382.1062
 406.5008 491.1997 598.9136
 697.8804 845.4810 875.5433
 1035.1886 1085.3853 1106.3828
 1186.2464 1231.4916 1247.5026
 1328.1602 1346.7081 1437.1728
 1520.3839 1571.6984 1578.7036
 1645.0584 1662.9837 3101.6282
 3114.7106 3156.4376 3184.6266
 3629.7816 3700.3833 3722.3143
 3892.4646 3957.8653 3965.7069

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Cartesian Coordinates

C -1.971647 0.356917 0.250804
 C -0.882811 -0.654918 -0.025545
 H -1.643512 1.346954 -0.078549
 O -3.122259 -0.076950 -0.480725
 H -2.170763 0.390293 1.325123
 H -0.656110 -0.673772 -1.093891
 O 0.262347 -0.249918 0.734391
 H -3.836082 0.556200 -0.337951
 H -1.219866 -1.646594 0.282815
 H 0.997021 -0.862161 0.539531
 O 2.111171 1.586844 -0.234406
 H 2.337113 2.381275 0.260715
 H 1.314268 1.208226 0.186979
 O 2.698041 -1.151403 -0.275272
 H 3.520179 -1.579604 -0.014863
 H 2.890106 -0.201397 -0.373366

Vibrational Frequencies

23.7095 35.8176 58.5466
 106.7566 162.8021 172.1247
 186.5291 193.5069 222.3297
 236.1023 315.2139 365.9706
 456.2753 492.0511 560.0637
 697.0404 843.3343 870.0850
 1033.1620 1085.0196 1105.6849
 1186.9197 1228.6795 1248.0603
 1327.8844 1339.6631 1432.2516
 1517.4618 1571.6756 1578.7492
 1644.3000 1668.4587 3100.3203
 3119.0274 3155.4131 3187.4192
 3630.4237 3700.5368 3732.2491
 3892.8709 3960.8311 3968.9916

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Cartesian Coordinates

C	-2.177905	0.391877	0.395777
C	-0.935501	-0.357129	0.832664
H	-1.937051	1.451581	0.249541
O	-2.715201	-0.172996	-0.795930
H	-2.956033	0.317748	1.155496
H	-1.174189	-1.405857	1.002552
O	0.039633	-0.339877	-0.221736
H	-1.968286	-0.274175	-1.404711
H	-0.522405	0.070458	1.751021
H	0.484779	0.530783	-0.223943
O	2.700227	-1.152890	0.016340
H	3.090529	-1.806354	-0.574008
H	1.732282	-1.216433	-0.094913
O	2.078560	1.555687	-0.186819
H	2.459623	2.237739	0.376172
H	2.645429	0.766621	-0.102691

Vibrational Frequencies

28.2326	39.0867	79.2962
127.8621	177.2430	203.7136
205.8780	236.7588	250.8775
346.5774	379.8514	406.8035
457.3930	544.2958	632.2924
689.9207	860.7132	899.5667
913.2542	1075.6698	1124.6373
1132.8729	1225.7777	1274.5337
1388.2379	1421.0072	1452.4776
1467.1109	1539.9358	1551.1835
1643.7934	1663.7301	3085.8436
3115.3345	3189.7075	3210.7078
3640.7445	3689.1406	3714.0404
3836.1411	3959.6809	3964.8867

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Cartesian Coordinates

C	-0.843775	-0.618697	-0.145146
C	-2.006148	0.201808	0.392386
H	-0.594254	-0.294393	-1.162065
O	0.298084	-0.515744	0.709554
H	-1.121583	-1.670585	-0.176723
H	-1.710309	1.252097	0.482842
O	-3.169119	0.060701	-0.428342
H	0.646940	0.393397	0.630719
H	-2.288285	-0.160687	1.378253
H	-2.996891	0.489815	-1.276415
O	2.901728	-0.936254	-0.224536
H	3.173474	-1.654931	-0.804713
H	2.012414	-1.158556	0.111862
O	1.859542	1.640642	-0.133899
H	2.341346	2.364334	0.281042
H	2.514799	0.946082	-0.330461

Vibrational Frequencies

23.7938	47.5653	63.4241
139.4879	153.8557	178.5074
200.0361	226.0795	260.0335
281.6596	316.9852	369.3518
426.4972	491.6093	600.7838
674.9678	820.8698	888.2616
1052.3209	1081.0537	1103.1135
1119.8305	1190.2427	1329.2256
1365.2112	1397.4477	1453.4234
1467.1635	1550.9257	1562.8037
1647.7343	1671.1802	3090.9420
3105.0677	3204.5927	3224.9755
3645.5793	3692.2989	3722.6508
3874.9381	3961.2172	3965.4577

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Cartesian Coordinates

C	1.131661	-0.422311	-0.639426
C	1.119571	0.369584	0.652383
H	2.085003	-0.296517	-1.156380
O	0.926712	-1.792612	-0.260427
H	0.325722	-0.072949	-1.287194
H	2.056410	0.234233	1.194206
O	0.943370	1.753913	0.282601
H	1.087472	-2.355369	-1.028790
H	0.290297	0.030584	1.274171
H	1.193300	2.306811	1.034153
O	-1.939031	-1.383253	0.644967
H	-1.991856	-0.524269	0.198474
H	-1.082306	-1.746779	0.380413
O	-1.703486	1.299733	-0.627958
H	-2.397614	1.966378	-0.669415
H	-0.894340	1.751988	-0.330846

Vibrational Frequencies

46.0737	89.0075	115.3388
126.3412	150.9686	164.3934
177.8106	204.4380	268.8484
302.8810	318.2811	415.5300
482.5273	488.0070	556.8449
565.2604	655.9240	853.0084
1015.8823	1059.8716	1090.4143
1151.3005	1234.3044	1248.2524
1309.5907	1338.7151	1422.1785
1511.0672	1570.2066	1580.0603
1660.5550	1692.8954	3124.2795
3135.9188	3184.8251	3209.9534
3720.6828	3781.4670	3883.3374
3884.4881	3904.1597	3963.6259

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Cartesian Coordinates

C -1.279584 -0.165657 -0.570342
 C -0.719955 -0.973389 0.594540
 H -2.027720 -0.745329 -1.114682
 O -1.926673 1.008145 -0.101842
 H -0.465168 0.074579 -1.259692
 H -1.523046 -1.415637 1.186400
 O 0.199467 -1.996469 0.148740
 H -1.209308 1.633310 0.102372
 H -0.132149 -0.324814 1.239402
 H -0.277585 -2.626636 -0.407692
 O 2.308822 -0.190232 -0.198328
 H 2.998282 -0.362212 -0.848664
 H 1.739199 -0.983085 -0.179543
 O 0.716754 2.109460 0.190734
 H 1.137981 2.736178 0.788526
 H 1.369782 1.400689 0.033952

Vibrational Frequencies

50.1835 74.4747 137.5521
 145.0785 172.5359 181.2850
 195.7686 202.3030 235.4201
 283.0945 345.9149 433.9145
 466.4067 480.3811 615.9888
 639.7341 760.5010 817.5084
 1026.2434 1076.8712 1110.8303
 1115.6094 1170.4775 1325.6616
 1350.7110 1397.7052 1457.9103
 1465.4836 1552.8957 1562.9173
 1673.8829 1691.6045 3110.0130
 3145.0430 3175.4540 3236.0646
 3651.8550 3691.4710 3759.3266
 3870.7635 3958.5282 3960.0696

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Cartesian Coordinates

C 1.497780 0.044869 -0.519293
 C 1.106966 -0.225299 0.926962
 H 1.048341 0.975474 -0.861378
 O 2.911022 0.221606 -0.655061
 H 1.133574 -0.765678 -1.157905
 H 1.474457 0.584571 1.561523
 O -0.306700 -0.385317 1.066219
 H 3.342810 -0.621783 -0.467074
 H 1.553209 -1.158181 1.274278
 H -0.734815 0.473119 0.881560
 O -2.469744 -1.159698 -0.542469
 H -2.438853 -1.826104 -1.236824
 H -1.660798 -1.267985 -0.008190
 O -1.927977 1.544850 -0.131960
 H -2.612277 2.155262 0.163361
 H -2.386926 0.762358 -0.489197

Vibrational Frequencies

26.4856 40.4686 75.3239
 144.7283 162.5866 180.8657
 211.2493 225.9120 254.8683
 285.5426 317.6669 363.2042
 413.8748 481.8511 576.9425
 690.7313 811.7930 851.7801
 1046.4099 1085.5521 1106.5547
 1120.5441 1186.6880 1339.2466
 1355.0748 1393.5677 1459.0726
 1466.3387 1552.5672 1564.8128
 1648.6404 1672.1109 3108.7703
 3123.4417 3185.6621 3216.4793
 3655.3463 3702.9712 3722.8458
 3873.6520 3960.5694 3965.4181

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Cartesian Coordinates

C -0.918728 -0.566301 -0.149887
 C -2.058249 0.293089 0.349377
 H -0.778666 -0.402351 -1.221618
 O 0.245346 -0.181788 0.588491
 H -1.152157 -1.619840 0.014728
 H -1.787793 1.348482 0.250819
 O -3.193980 -0.027707 -0.460270
 H 0.961384 -0.821457 0.410136
 H -2.243757 0.076692 1.404138
 H -3.968526 0.418338 -0.097044
 O 2.714705 -1.212908 -0.207436
 H 2.941883 -0.268253 -0.287531
 H 3.445101 -1.634243 0.258085
 O 2.332278 1.550422 -0.091034
 H 1.436532 1.249929 0.157049
 H 2.221073 2.267823 -0.723713

Vibrational Frequencies

26.3347 36.1094 57.7972
 119.5533 161.9825 181.1525
 201.5529 208.7273 216.6221
 253.8044 318.0532 365.3274
 421.5377 500.0582 599.4617
 690.7328 842.0560 886.9687
 1035.2618 1084.6536 1105.9702
 1178.8288 1234.1970 1246.2557
 1327.3601 1340.6129 1431.9339
 1516.3492 1570.5763 1578.5612
 1651.2330 1674.2475 3101.4765
 3113.6468 3157.0708 3184.7654
 3642.6690 3693.4871 3721.4325
 3893.0050 3962.4012 3963.3831

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Cartesian Coordinates

C	1.135480	-0.838791	-0.562672
C	1.185080	0.446564	0.234277
H	1.570092	-1.651631	0.021366
O	-0.255121	-1.114380	-0.852264
H	1.696891	-0.720932	-1.490218
H	0.587832	0.343595	1.142559
O	2.570667	0.642946	0.537915
H	-0.295333	-1.861544	-1.464138
H	0.783056	1.269873	-0.358266
H	2.662677	1.479695	1.009838
O	-2.019102	1.473369	-0.818384
H	-2.232244	1.080590	0.041373
H	-1.543741	0.762899	-1.267023
O	-1.937240	-0.526330	1.370608
H	-1.439825	-1.017189	0.695253
H	-2.586392	-1.136829	1.736637

Vibrational Frequencies

35.7167	45.4778	68.3879
70.4199	117.6058	161.4905
184.3824	188.2226	207.5261
288.2915	304.8275	306.5715
378.5818	442.7197	487.0517
565.6536	629.2938	848.1005
1007.8196	1065.6762	1092.1128
1175.6309	1204.8064	1251.8479
1300.6771	1339.6172	1422.2225
1515.3113	1571.1390	1584.2880
1637.8719	1694.4854	3125.1991
3132.4027	3183.5246	3207.3450
3746.6156	3813.7867	3874.6093
3892.5758	3940.0862	3965.1802

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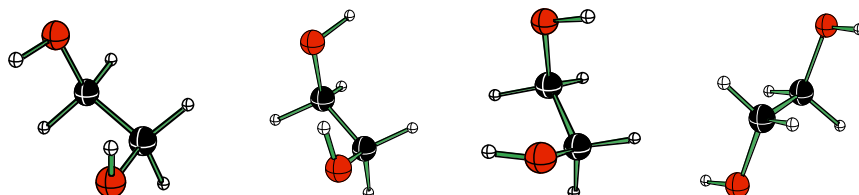
Cartesian Coordinates

C	-0.899320	-0.576612	-0.199086
C	-2.027199	0.276801	0.361192
H	-0.716190	-0.303118	-1.241493
O	0.285310	-0.444480	0.590538
H	-1.172919	-1.632046	-0.161852
H	-1.761268	1.331400	0.303514
O	-3.222193	0.139189	-0.413684
H	0.653646	0.449707	0.447412
H	-2.194585	0.020815	1.410688
H	-3.575722	-0.748224	-0.271432
O	2.942067	-1.009092	-0.100083
H	3.202589	-1.713850	-0.702255
H	2.012118	-1.175123	0.146241
O	1.996823	1.609087	-0.186994
H	2.453931	2.327345	0.263521
H	2.641451	0.884330	-0.285193

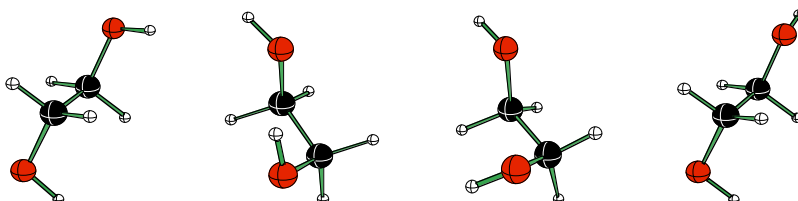
Vibrational Frequencies

23.2126	46.1736	65.5724
139.0245	153.9760	185.8662
201.0054	226.4701	258.2180
279.6383	314.0918	368.5904
422.7530	492.6253	594.3490
689.2142	819.7961	891.3559
1051.5669	1084.3294	1101.8577
1122.9979	1186.5630	1342.8990
1355.5470	1393.1056	1455.3153
1465.9539	1551.4153	1563.4825
1648.8567	1671.9585	3115.4753
3123.5521	3182.0290	3212.0117
3640.2447	3689.6160	3720.6931
3877.3042	3962.7747	3964.1750

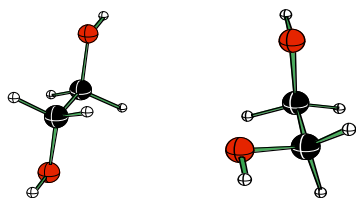
S.2.



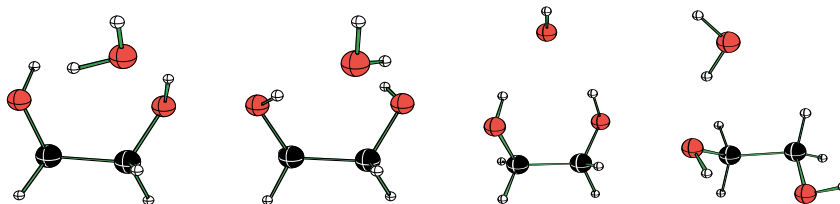
Complex #	mpm - TS	ppm	ppp	ptm
E MP2/6-31+G**	-229.618051	-229.619048	-229.614321	-229.614965
E B3LYP/6-311+G**	-230.336014	-230.337115	-230.333138	-230.333608
Raw ZPE	0.086827	0.087534	0.086650	0.087099
Thermal Corr. H(298)	0.092358	0.093399	0.093048	0.093314
Thermal Corr. G(298)	0.060483	0.060390	0.059285	0.059607
State	1-A		1-A	1-AG
Point Group	C2	C1	C2	CI
Nimag	1	0	0	0
Rotational Constant	14.95096	15.04836	15.09087	29.42053
Rotational Constant	5.54560	5.59688	5.41634	3.88545
Rotational Constant	4.54008	4.62497	4.51600	3.65267



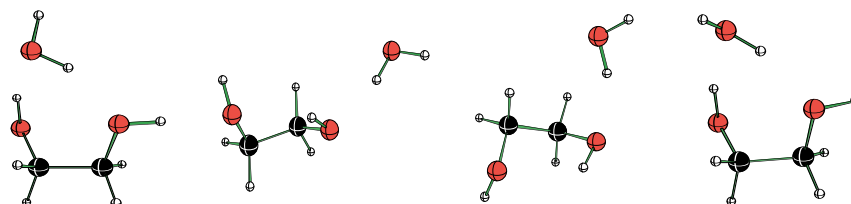
Complex #	ptp	tpm	tpp	ttp
E MP2/6-31+G**	-229.614425	-229.620175	-229.613089	-229.614962
E B3LYP/6-311+G**	-230.333153	-230.337881	-230.331895	-230.333466
Raw ZPE	0.087051	0.087458	0.086690	0.086833
Thermal Corr. H(298)	0.093257	0.093394	0.092965	0.093185
Thermal Corr. G(298)	0.060236	0.060257	0.058990	0.059124
State	1-A			
Point Group	C2	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	29.39922	15.17127	16.12574	29.85005
Rotational Constant	3.88853	5.67812	5.16123	3.94735
Rotational Constant	3.65485	4.66179	4.46293	3.68396



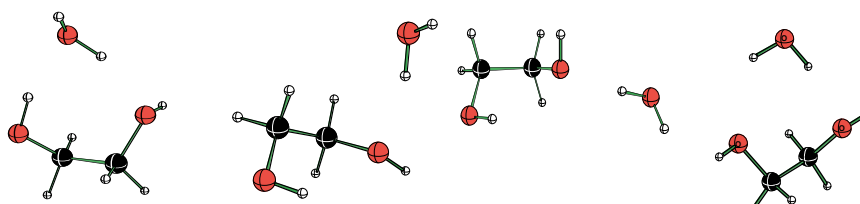
Complex #	ttt	tpt
E MP2/6-31+G**	-229.615397	-229.613720
E B3LYP/6-311+G**	-230.333727	-230.332217
Raw ZPE	0.086531	0.086592
Thermal Corr. H(298)	0.093091	0.092935
Thermal Corr. G(298)	0.059043	0.059489
State	1-AG	1-A
Point Group	C2H	C2
Nimag	0	0
Rotational Constant	30.33629	16.68899
Rotational Constant	4.01321	5.14104
Rotational Constant	3.71011	4.48784



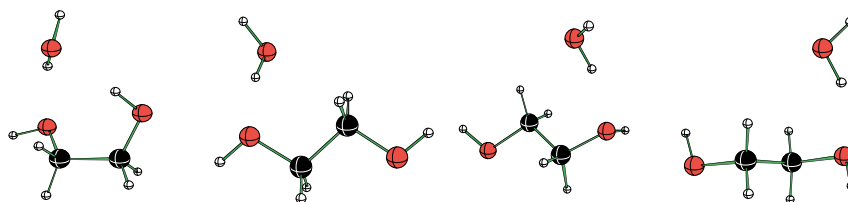
Complex #	1 (mpm)	22 (mmm)	29 (pmp)	62 (tpm)
E MP2/6-31+G**	-305.868317	-305.864908	-305.865052	-305.866673
E B3LYP/6-311+G**	-306.809091	-306.806841	-306.806917	-306.807633
Raw ZPE	0.113243	0.113087	0.112400	0.112593
Thermal Corr. H(298)	0.121976	0.121770	0.121678	0.121710
Thermal Corr. G(298)	0.082045	0.082022	0.080109	0.079950
State			1-A	
Point Group	C1	C1	C2	C1
Nimag	0	0	0	0
Rotational Constant	4.96637	4.93273	5.23852	5.93036
Rotational Constant	3.48580	3.51660	2.98875	2.47386
Rotational Constant	2.41838	2.40851	2.02380	2.14815



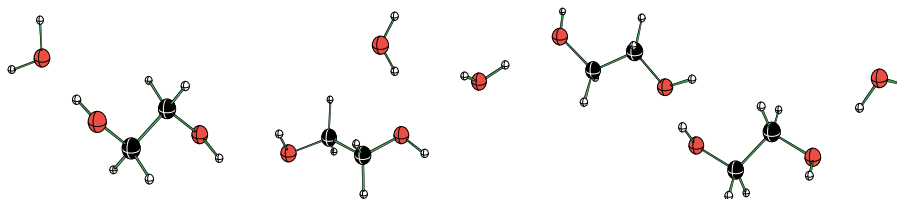
Complex #	89 (tpm)	94 (ppm)	103 (ppm)	105 (tpm)
E MP2/6-31+G**	-305.867484	-305.863488	-305.865093	-305.869479
E B3LYP/6-311+G**	-306.810031	-306.805824	-306.805915	-306.810384
Raw ZPE	0.112981	0.112460	0.112463	0.113174
Thermal Corr. H(298)	0.121733	0.121680	0.121603	0.121845
Thermal Corr. G(298)	0.081562	0.078784	0.079711	0.081936
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	4.93342	9.76165	6.60376	4.91349
Rotational Constant	3.48137	1.71857	2.29691	3.48632
Rotational Constant	2.23474	1.65635	2.07028	2.22241



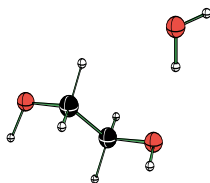
Complex #	106 (pmm)	112 (tmp)	121 (pmm)	126 (tpt)
E MP2/6-31+G**	-305.867871	-305.863241	-305.863734	-305.861403
E B3LYP/6-311+G**	-306.809915	-306.805180	-306.804696	-306.803018
Raw ZPE	0.113270	0.112144	0.112161	0.111931
Thermal Corr. H(298)	0.121859	0.121552	0.121548	0.121392
Thermal Corr. G(298)	0.082038	0.078244	0.078000	0.078805
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	4.91261	6.74625	10.67996	5.00817
Rotational Constant	3.42868	2.15249	1.59616	3.16002
Rotational Constant	2.17057	1.96446	1.53250	2.09470



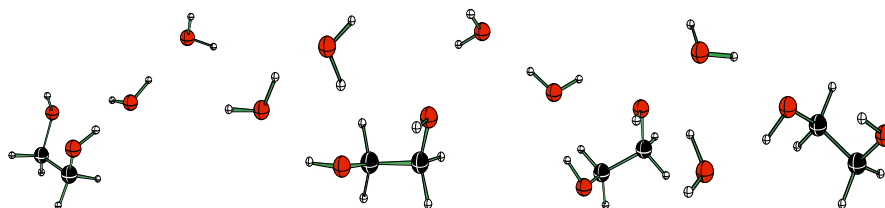
Complex #	129 (tpp)	135 (ttt)	143 (ttm)	153 (ptm)
E MP2/6-31+G**	-305.863226	-305.860608	-305.860919	-305.860272
E B3LYP/6-311+G**	-306.804525	-306.801960	-306.802329	-306.802166
Raw ZPE	0.112881	0.111709	0.111880	0.111935
Thermal Corr. H(298)	0.121675	0.121435	0.121461	0.121455
Thermal Corr. G(298)	0.081514	0.077926	0.078679	0.078857
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	4.89299	6.04870	6.00412	5.63955
Rotational Constant	3.54042	2.21000	2.24176	2.38211
Rotational Constant	2.33640	1.70930	1.73843	1.82054



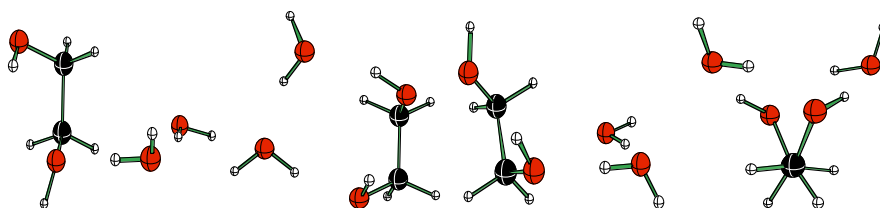
Complex #	159 (mtp)	162 (ttp)	169 (tpp)	171 (ptp)
E MP2/6-31+G**	-305.859622	-305.859710	-305.859562	-305.858966
E B3LYP/6-311+G**	-306.802183	-306.801738	-306.801554	-306.801175
Raw ZPE	0.111514	0.111956	0.111465	0.111798
Thermal Corr. H(298)	0.121479	0.121486	0.121359	0.121480
Thermal Corr. G(298)	0.076993	0.078668	0.076526	0.077310
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	6.59997	5.59022	14.53997	14.03153
Rotational Constant	1.91564	2.41731	1.35944	1.37981
Rotational Constant	1.58799	1.84319	1.28612	1.29007



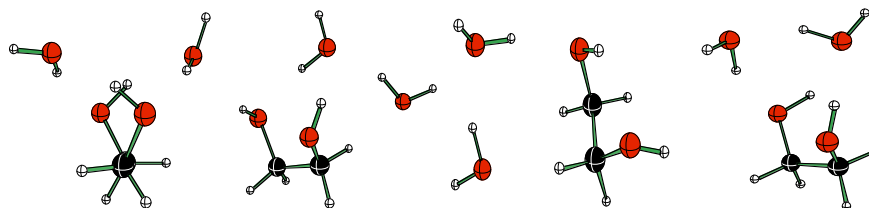
Complex #	172 (mtm)
E MP2/6-31+G**	-305.859231
E B3LYP/6-311+G**	-306.801135
Raw ZPE	0.111858
Thermal Corr. H(298)	0.121420
Thermal Corr. G(298)	0.078490
State	
Point Group	C1
Nimag	0
Rotational Constant	6.02867
Rotational Constant	2.18120
Rotational Constant	1.70561



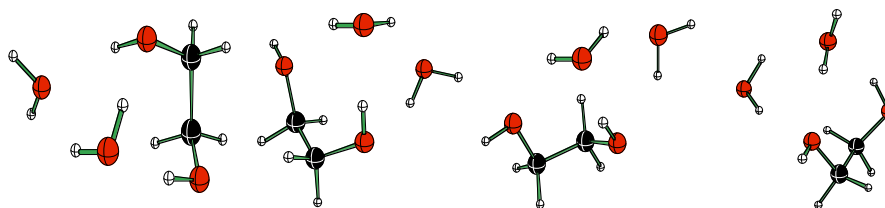
Conformation #	100 (mpm)	102 (tmp)	104 (pmp)	105 (mmp)
E MP2/6-31+G**	-382.111869	-382.116559	-382.111924	-382.116613
E B3LYP/6-311+G**	-383.277921	-383.281372	-383.278133	-383.283013
Raw ZPE	0.137721	0.13854	0.137702	0.138604
Thermal Corr. H(298)	0.150152	0.150239	0.150101	0.150312
Thermal Corr. G(298)	0.099063	0.102513	0.098918	0.101578
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	4.92019	3.93348	4.55854	4.59649
Rotational Constant	0.9663	1.5836	0.98674	1.13997
Rotational Constant	0.8601	1.22845	0.88857	1.02192



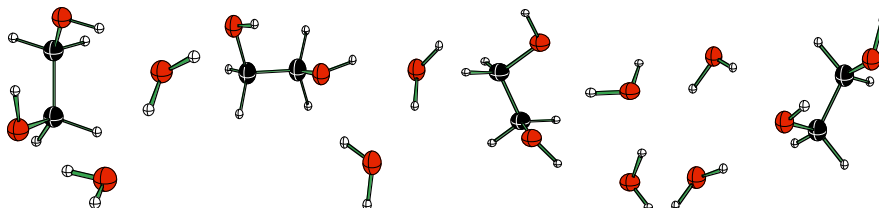
Conformation #	107 (tmp)	10 (mpm)	114 (tmp)	118 (mmm)
E MP2/6-31+G**	-382.112381	-382.122750	-382.115821	-382.118876
E B3LYP/6-311+G**	-383.277773	-383.288044	-383.281132	-383.283393
Raw ZPE	0.137853	0.139491	0.138062	0.139712
Thermal Corr. H(298)	0.149965	0.150661	0.150057	0.150695
Thermal Corr. G(298)	0.10055	0.104382	0.100922	0.106359
State				1-A
Point Group	C1	C1	C1	C2
Nimag	0	0	0	0
Rotational Constant	3.27551	2.90752	3.27805	2.67835
Rotational Constant	1.47775	2.0826	1.55911	2.05872
Rotational Constant	1.26359	1.39254	1.23358	1.92288



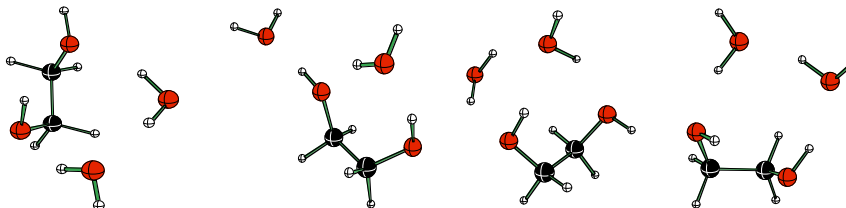
Conformation #	119 (pmp)	97 (mpm)	122 (pmm)	123 (ppm)
E MP2/6-31+G**	-382.121474	-382.112024	-382.113713	-382.118996
E B3LYP/6-311+G**	-383.286134	-383.277386	-383.279191	-383.284413
Raw ZPE	0.13968	0.138181	0.137921	0.139228
Thermal Corr. H(298)	0.150677	0.150221	0.149939	0.150456
Thermal Corr. G(298)	0.105572	0.101018	0.100858	0.104066
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	2.55722	2.96433	3.32892	3.17513
Rotational Constant	2.15555	1.62412	1.54348	1.87288
Rotational Constant	1.93596	1.46477	1.22203	1.50585



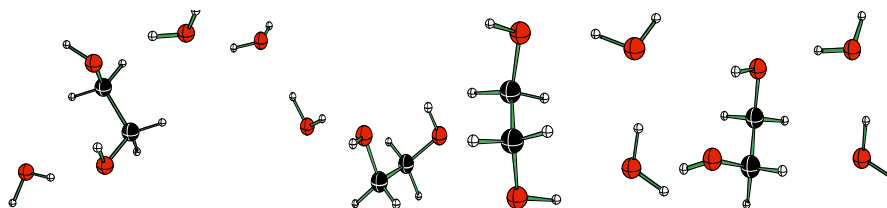
Conformation #	125 (mmp)	126 (tmp)	127 (tpm)	129 (tpm)
E MP2/6-31+G**	-382.110601	-382.116807	-382.115285	-382.111832
E B3LYP/6-311+G**	-383.276607	-383.282714	-383.280863	-383.276944
Raw ZPE	0.138065	0.139005	0.138545	0.138171
Thermal Corr. H(298)	0.150096	0.150363	0.150136	0.150038
Thermal Corr. G(298)	0.101161	0.103705	0.103018	0.102135
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	-	0
Rotational Constant	2.90851	2.93536	3.60966	2.80199
Rotational Constant	1.76267	1.88181	1.72622	1.89813
Rotational Constant	1.43734	1.65136	1.32484	1.54166



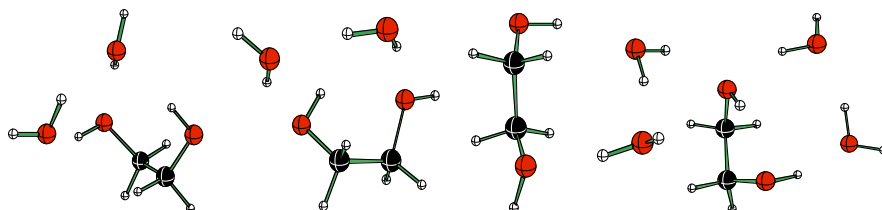
Conformation #	132 (mpp)	134 (tpm)	136 (tpt)	144 (tpm)
E MP2/6-31+G**	-382.121171	-382.116778	-382.116697	-382.111050
E B3LYP/6-311+G**	-383.286157	-383.283112	-383.281786	-383.275756
Raw ZPE	0.139567	0.138537	0.138275	0.137201
Thermal Corr. H(298)	0.150703	0.150264	0.15008	0.149706
Thermal Corr. G(298)	0.104766	0.101442	0.102204	0.098905
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	3.07295	4.51489	3.70335	4.18684
Rotational Constant	2.02903	1.12624	1.69272	1.34555
Rotational Constant	1.41123	1.01155	1.27139	1.14382



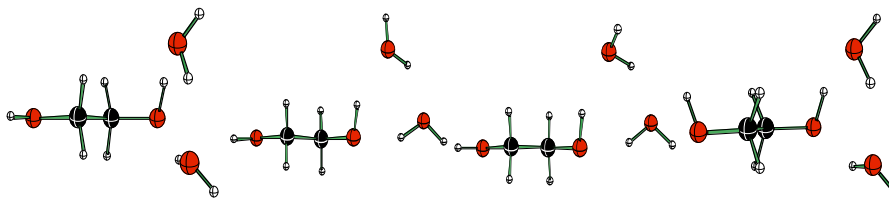
Conformation #	149 (tpm)	155 (tmp)	157 (ppm)	160 (mpm)
E MP2/6-31+G**	-382.111451	-382.113590	-382.112895	-382.122473
E B3LYP/6-311+G**	-383.276498	-383.280149	-383.278240	-383.287601
Raw ZPE	0.138481	0.137442	0.138271	0.139213
Thermal Corr. H(298)	0.150238	0.149925	0.150024	0.150534
Thermal Corr. G(298)	0.102493	0.099018	0.102514	0.103844
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	3.07276	3.38834	2.72923	2.8987
Rotational Constant	1.81083	1.33778	1.97879	2.09687
Rotational Constant	1.31805	1.02687	1.60004	1.39243



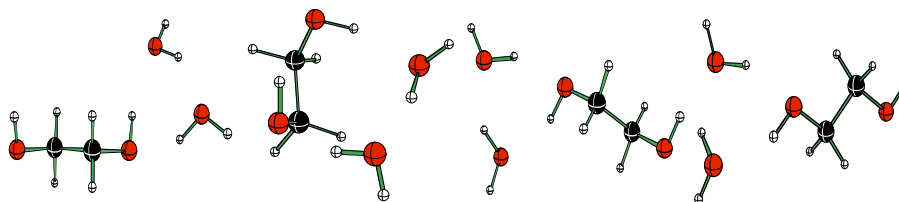
Conformation #	162 (tpm)	163 (tpm)	167 (mtp)	170 (mpp)
E MP2/6-31+G**	-382.110204	-382.105776	-382.115912	-382.114224
E B3LYP/6-311+G**	-383.275161	-383.271986	-383.281192	-383.279776
Raw ZPE	0.137204	0.136819	0.138861	0.138063
Thermal Corr. H(298)	0.149788	0.149776	0.150395	0.150005
Thermal Corr. G(298)	0.098359	0.09608	0.103535	0.101277
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	5.31047	4.79635	2.5001	3.35287
Rotational Constant	1.19032	0.81945	2.29048	1.53684
Rotational Constant	1.08622	0.77997	1.30769	1.22169



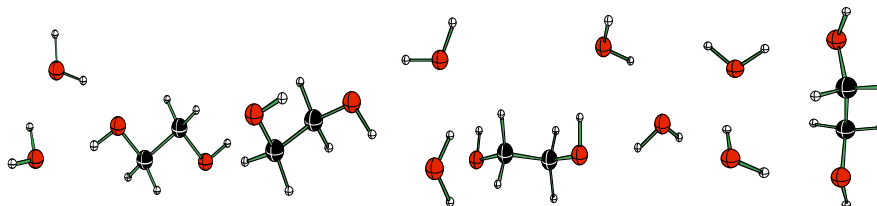
Conformation #	175 (mmp)	176 (tpm)	179 (ttm)	182 (mmp)
E MP2/6-31+G**	-382.118651	-382.111371	-382.115717	-382.121301
E B3LYP/6-311+G**	-383.284238	-383.2762556	-383.280768	-383.286427
Raw ZPE	0.139062	0.138482	0.138757	0.139744
Thermal Corr. H(298)	0.150359	0.150264	0.150378	0.150759
Thermal Corr. G(298)	0.104156	0.101876	0.10319	0.10516
State		1-A		
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	2.97883	2.9686	2.50638	3.07792
Rotational Constant	1.89164	1.87432	2.28509	2.01178
Rotational Constant	1.61081	1.29884	1.31136	1.4058



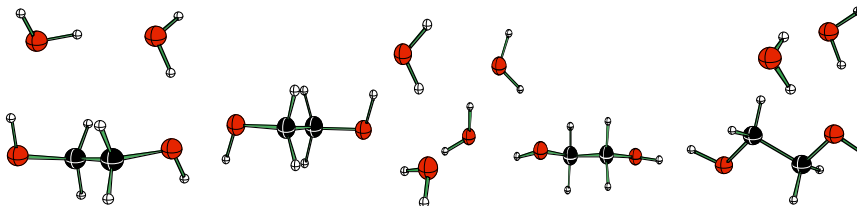
Conformation #	184 (ttm)	189 (ttm)	192 (ttm)	195 (mtm)
E MP2/6-31+G**	-382.112529	-382.112100	-382.111991	-382.112034
E B3LYP/6-311+G**	-383.278954	-383.279329	-383.278998	-383.278659
Raw ZPE	0.138003	0.137977	0.137777	0.138091
Thermal Corr. H(298)	0.150081	0.150121	0.15004	0.150108
Thermal Corr. G(298)	0.101015	0.100257	0.099954	0.101182
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	3.64323	5.13699	5.02658	3.61377
Rotational Constant	1.2701	1.0179	1.04335	1.26481
Rotational Constant	1.21793	0.90069	0.9225	1.21559



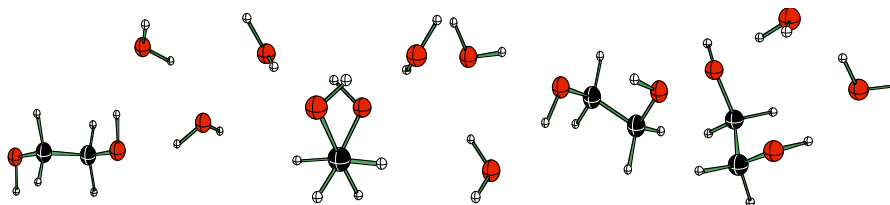
Conformation #	199 (ptp)	1 (mpp)	201 (ptm)	202 (ttt)
E MP2/6-31+G**	-382.112187	-382.121300	-382.111918	-382.111794
E B3LYP/6-311+G**	-383.279060	-383.286468	-383.279175	-383.278864
Raw ZPE	0.138166	0.13973	0.138242	0.137785
Thermal Corr. H(298)	0.150183	0.150756	0.150235	0.15001
Thermal Corr. G(298)	0.100822	0.10513	0.100887	0.099663
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	4.79672	3.0787	5.0509	4.95077
Rotational Constant	1.08232	2.00886	1.02793	1.04884
Rotational Constant	0.95831	1.40367	0.90783	0.92405



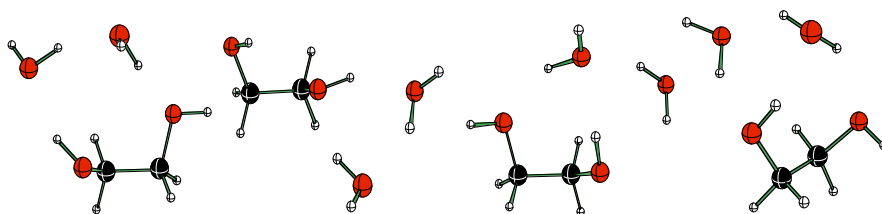
Conformation #	203 (ttt)	206 (mpp)	211 (mtm)	212 (ttt)
E MP2/6-31+G**	-382.111693	-382.116499	-382.112021	-382.107613
E B3LYP/6-311+G**	-383.278620	-383.283078	-383.278907	-383.272445
Raw ZPE	0.137634	0.138619	0.138155	0.138193
Thermal Corr. H(298)	0.14995	0.150303	0.1502	0.150154
Thermal Corr. G(298)	0.099355	0.101664	0.100647	0.10219
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	4.85546	4.5824	4.92437	2.33919
Rotational Constant	1.06844	1.13597	1.06432	2.25484
Rotational Constant	0.93701	1.01886	0.94216	1.35975



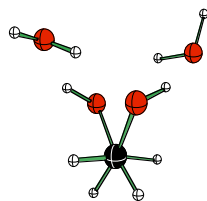
Conformation #	215 (mtp)	220 (mtp)	221 (ttt)	224 (ttt)
E MP2/6-31+G**	-382.115293	-382.111563	-382.111683	-382.104422
E B3LYP/6-311+G**	-383.280582	-383.278411	-383.278748	-383.270138
Raw ZPE	0.138457	0.138121	0.137823	0.136861
Thermal Corr. H(298)	0.150204	0.150151	0.15003	0.149645
Thermal Corr. G(298)	0.102799	0.100791	0.099823	0.098541
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	2.4962	3.88541	5.141	3.06878
Rotational Constant	2.2833	1.17993	1.00942	1.37511
Rotational Constant	1.29793	1.1138	0.89098	1.31075



Conformation #	225 (mtp)	24 (mpm)	34 (mmp)	41 (tmm)
E MP2/6-31+G**	-382.111809	-382.121609	-382.116670	-382.117238
E B3LYP/6-311+G**	-383.278967	-383.2861203	-383.282984	-383.282505
Raw ZPE	0.138184	0.139712	0.138539	0.13914
Thermal Corr. H(298)	0.150224	0.150695	0.15027	0.150456
Thermal Corr. G(298)	0.100651	0.106359	0.101642	0.104104
State		1-A		
Point Group	C1	C2	C1	C1
Nimag	0	0	0	0
Rotational Constant	5.17471	2.67835	4.62832	2.90977
Rotational Constant	1.02115	2.05872	1.15745	1.9983
Rotational Constant	0.90012	1.92288	1.03107	1.61395



Conformation #	87 (tmt)	48 (tpm)	58 (tpm)	63 (mpp)
E MP2/6-31+G**	-382.116641	-382.116853	-382.112407	-382.116248
E B3LYP/6-311+G**	-383.282931	-383.283047	-383.277822	-383.282359
Raw ZPE	0.13835	0.138473	0.137806	0.138912
Thermal Corr. H(298)	0.150101	0.15022	0.149858	0.150257
Thermal Corr. G(298)	0.101964	0.101445	0.101256	0.103672
State				
Point Group	C1	C1	C1	C1
Nimag	0	0	0	0
Rotational Constant	3.12067	4.57969	3.39032	3.01261
Rotational Constant	1.86808	1.14928	1.69446	1.87311
Rotational Constant	1.30396	1.02586	1.31037	1.53225



Conformation #	65 (mmm)
E MP2/6-31+G**	-382.118576
E B3LYP/6-311+G**	-383.283277
Raw ZPE	0.139556
Thermal Corr. H(298)	0.150504
Thermal Corr. G(298)	0.105566
State	
Point Group	C1
Nimag	0
Rotational Constant	2.62419
Rotational Constant	2.1121
Rotational Constant	1.92321

S.3.

Table 1. Relative Energies (kcal/mol) and Boltzmann Weightings for MP2/6-31+G** Ethylene Glycol in the gas phase.

Conformation	Deg.	MP2/6-31+G**			B3LYP/6-311+G** ^a		
		$\Delta H(0)^b$	$\Delta G(298)^c$	%	$\Delta H(0)^b$	$\Delta G(298)^c$	%
tG+g-	4	0.0	0.0	77.3	0.0	0.0	68.5
g+G+g-	4	0.8	0.8	20.4	0.5	0.6	26.5
g-G+g-	2	1.0	1.5	0	0.8	1.3	0
tTg+	4	2.9	2.6	1.0	2.4	2.1	2.1
g+Tg-	2	3.1	2.9	0.3	2.5	2.3	0.7
g+G+g+	2	3.2	3.1	0.2	2.5	2.4	0.6
tG+g+	4	4.0	3.7	0.2	3.3	3.0	0.5
g+Tg+	2	3.4	3.6	0.1	2.7	3.0	0.2
tTt	1	2.4	2.3	0.4	2.0	1.9	0.7
tG+t	2	3.5	3.6	0.1	3.0	3.1	0.2

a. Sum of electronic and zero-point vibrational energy

b. Free energy values do not account for the contribution of the degeneracy to the entropy term.

c. Values correspond to B3LYP/6-311+G** energies for MP2/6-31+G** geometries.

Table 2. Relative Energies (kcal/mol) and Boltzmann Weightings for MP2/6-31+G** Ethylene Glycol 1 Water Complexes.

1 water complexes		Degeneracy			MP2/6-31+G**			B3LYP/6-311+G** ^a		
#	EG	EG	EG w/1W	Total ^b	$\Delta H(0)^c$	$\Delta G(298)^d$	%	$\Delta H(0)^c$	$\Delta G(298)^d$	%
89	tG+g-	4	1	4	1.14	1.02	7.3	0.10	0.00	24.9
105	tG+g-	4	1	4	0.00	0.00	41.1	0.00	0.01	24.5
106	g+G+g-	4	1	4	1.07	1.07	6.7	0.35	0.36	13.4
62	tG+g-	4	1	4	1.41	0.53	16.8	1.38	0.50	10.6
1	g-G+g-	2	2	4	0.77	0.80	10.7	0.85	0.89	5.6
94	g+G+g-	4	1	4	3.33	1.80	2.0	2.43	0.91	5.4
112	tG+g-	4	1	4	3.29	1.62	2.7	2.64	0.98	4.7
121	g+G+g-	4	1	4	2.99	1.16	5.8	2.96	1.13	3.7
103	g+G+g-	4	1	4	2.32	1.37	4.0	2.38	1.43	2.2
29	g-G+g-	2	1	2	2.31	1.65	1.3	1.71	1.06	2.1
159	g+Tg-	2	2	4	5.18	3.12	0.2	4.14	2.09	0.7
169	tTg+	4	1	4	5.19	2.87	0.3	4.51	2.20	0.6
22	g+G+g+	2	2	4	2.82	2.92	0.3	2.17	2.29	0.5
126	tG+t	2	2	4	4.32	3.13	0.2	3.87	2.70	0.3
171	g+Tg+	2	2	4	5.77	3.73	0.1	4.95	2.92	0.2
143	tTg+	4	1	4	4.59	3.36	0.1	4.27	3.05	0.1
135	tTt	1	2	2	4.68	3.09	0.1	4.40	2.81	0.1
153	g+Tg-	2	2	4	5.03	3.88	0.1	4.41	3.26	0.1
162	tTg+	4	1	4	5.40	4.11	0.0	4.69	3.41	0.1
129	tG+g+	4	1	4	3.75	3.67	0.1	3.50	3.43	0.1
172	g+Tg+	2	2	4	5.64	4.30	0.0	5.01	3.68	0.0

a Total degeneracy is the product of EG and complex degeneracy.

b Sum of electronic and zero-point vibrational energy

c Free energy values do not account for the contribution of the degeneracy to the entropy term.

d Values correspond to B3LYP/6-311+G** energies for MP2/6-31+G** geometries.

Table 3. Relative Energies (kcal/mol) and Boltzmann Weightings for MP2/6-31+G** Ethylene Glycol 2 Water Complexes.

#	2 water complexes EG	Degeneracy			MP2/6-31+G**			B3LYP/6-311+G** ^a		
		EG	EG w/2W ^b	Total ^c	$\Delta H(0)$ ^d	$\Delta G(298)$ ^e	%	$\Delta H(0)$ ^d	$\Delta G(298)$ ^e	%
160	g-G+g-	4	2	8	0.0	0.0	42.5	0.0	0.0	34.2
10	g-G+g-	4	2	8	0.0	0.2	32.6	-0.1	0.1	31.3
134	tG+g-	4	2	8	3.1	2.1	1.3	2.4	1.3	3.6
48	tG+g-	4	2	8	3.1	2.0	1.4	2.4	1.4	3.4
105	g+G+g-	4	2	8	3.3	2.3	0.9	2.5	1.5	2.9
132	g+G+g-	4	2	8	1.0	1.4	4.1	1.1	1.5	2.8
206	g+G+g-	4	2	8	3.4	2.4	0.7	2.5	1.5	2.8
1	g+G+g-	4	2	8	1.1	1.5	3.2	1.0	1.5	2.7
34	g+G+g-	4	2	8	3.2	2.3	0.9	2.5	1.5	2.6
182	g+G+g-	4	2	8	1.1	1.5	3.1	1.1	1.5	2.5
155	tG+g-	4	2	8	4.5	2.6	0.5	3.6	1.7	2.0
87	tG+t	2	4	8	3.1	2.5	0.6	2.4	1.8	1.7
119	g-G+g-	2	4	8	0.9	1.7	2.4	1.2	2.0	1.2
123	g+G+g-	4	2	8	2.2	2.3	0.8	2.0	2.1	0.9
114	tG+g-	4	2	8	3.5	2.4	0.8	3.4	2.3	0.8
175	g+G+g-	4	2	8	2.3	2.6	0.5	2.0	2.3	0.7
24	g-G+g-	2	4	8	0.9	2.1	1.2	1.2	2.5	0.5
136	g+Tg+	2	4	8	3.0	2.6	0.5	3.1	2.6	0.4
104	g-G+g-	2	4	8	5.7	3.6	0.1	5.0	2.9	0.3
189	tTg+	4	2	8	5.7	4.3	0.0	4.4	3.0	0.2
126	tG+g-	4	2	8	3.4	3.5	0.1	2.9	3.0	0.2
192	tTg+	4	2	8	5.7	4.2	0.0	4.5	3.0	0.2
102	tG+g-	4	2	8	3.3	2.9	0.3	3.5	3.1	0.2
100	g-G+g-	2	4	8	5.7	3.7	0.1	5.2	3.1	0.2
63	g+G+g-	4	2	8	3.7	3.8	0.1	3.1	3.2	0.2
203	tTt	1	4	4	5.8	4.0	0.0	4.7	2.9	0.1
202	tTt	1	4	4	5.8	4.1	0.0	4.6	2.9	0.1
170	g+G+g-	4	2	8	4.5	3.6	0.1	4.2	3.3	0.1
41	tG+g+	4	2	8	3.2	3.4	0.1	3.2	3.4	0.1
122	g+G+g-	4	2	8	4.7	3.7	0.1	4.5	3.4	0.1
225	g+Tg-	2	4	8	6.0	4.7	0.0	4.8	3.4	0.1
201	g+Tg-	2	4	8	6.0	4.8	0.0	4.7	3.5	0.1
211	g+Tg+	2	4	8	5.9	4.6	0.0	4.8	3.5	0.1
221	tTt	1	4	4	5.9	4.3	0.0	4.7	3.1	0.1
199	g+Tg+	2	4	8	5.8	4.6	0.0	4.7	3.5	0.1
184	tTg+	4	2	8	5.5	4.5	0.0	4.7	3.7	0.1
127	tG+g-	4	2	8	4.1	4.0	0.0	3.8	3.7	0.1
215	g+Tg-	2	4	8	4.0	3.9	0.1	3.9	3.8	0.1
65	g+G+g+	2	4	8	2.7	3.5	0.1	2.9	3.8	0.1
167	g+Tg-	2	4	8	3.9	3.9	0.1	3.8	3.8	0.1
220	g+Tg-	2	4	8	6.2	5.0	0.0	5.1	3.9	0.0
179	tTg+	4	2	8	4.0	3.8	0.1	4.0	3.9	0.0
195	g+Tg+	2	4	8	5.8	4.9	0.0	4.9	4.0	0.0
107	tG+g-	4	2	8	5.5	4.3	0.0	5.3	4.1	0.0
144	tG+g-	4	2	8	5.9	4.1	0.0	6.2	4.4	0.0
162	tG+g-	4	2	8	6.4	4.3	0.0	6.6	4.4	0.0
58	tG+g-	4	2	8	5.4	4.7	0.0	5.3	4.5	0.0
97	g-G+g-	2	4	8	5.9	4.8	0.0	5.8	4.7	0.0
118	g+G+g+	2	2	4	2.5	3.9	0.0	2.9	4.3	0.0
163	tG+g-	4	2	8	9.0	5.7	0.0	8.4	5.0	0.0
157	g+G+g-	4	2	8	5.4	5.2	0.0	5.3	5.1	0.0
125	g+G+g-	4	2	8	6.7	5.8	0.0	6.2	5.2	0.0
129	tG+g-	4	2	8	6.0	5.6	0.0	6.1	5.6	0.0
176	tG+g-	4	2	8	6.5	5.7	0.0	6.7	5.9	0.0
149	tG+g-	4	2	8	6.5	6.1	0.0	6.5	6.1	0.0
224	tTt	1	4	4	9.9	8.1	0.0	9.5	7.7	0.0
212	tTt	1	4	4	8.7	8.3	0.0	8.9	8.5	0.0

^a Degeneracy includes exchange of waters and of complex degeneracy.

^b Total degeneracy is the product of EG and complex degeneracy.

^c Sum of electronic and zero-point vibrational energy

^d Free energy values do not account for the contribution of the degeneracy to the entropy term.

^e Values correspond to B3LYP/6-311+G** energies for MP2/6-31+G** geometries.

S.4.1. Boltzmann percentage for the unique conformational complexes of ethylene glycol complexed to one water molecule based on relative energies computed at the B3LYP/6-311+G**//MP2/6-31+G** level.

Complex #	$\Delta E_{\text{BW}}^{\text{a}}$	$\Delta H(0)^{\text{b}}$	$\Delta G(298)^{\text{c}}$
1	9.5	8.4	5.6
22	0.9	0.9	0.5
29	0.5	1.0	2.1
62	2.0	3.5	10.6
89	25.8	29.5	24.9
94	0.3	0.6	5.4
103	0.3	0.6	2.2
105	37.5	35.2	24.5
106	22.8	19.4	13.4
112	0.2	0.4	4.7
121	0.1	0.2	3.7
129	0.1	0.1	0.1
135	0.0	0.0	0.1
143	0.0	0.0	0.1
153	0.0	0.0	0.1
159	0.0	0.0	0.7
162	0.0	0.0	0.1
169	0.0	0.0	0.6
171	0.0	0.0	0.2
172	0.0	0.0	0.0
126	0.0	0.1	0.3

a. Percentage based on the relative bottom-of-the-well electronic energy.

b. Percentage based on the relative ZPVE corrected electronic energy (see methods section).

c. Percentage based on the relative 298 K free energy electronic energy.

S.4.2. Boltzmann percentage for the unique conformational complexes of ethylene glycol complexed to two water molecules based on relative energies computed at the B3LYP/6-311+G**//MP2/6-31+G** level.

Complex #	$\Delta E_{\text{BW}}^{\text{a}}$	$\Delta H(0)^{\text{b}}$	$\Delta G(298)^{\text{c}}$
100	0.0	0.0	0.2
102	0.0	0.1	0.2
104	0.0	0.0	0.3
105	0.2	0.5	2.9
107	0.0	0.0	0.0
10	40.2	37.9	31.3
114	0.0	0.1	0.8
118	0.1	0.1	0.0
119	5.3	4.1	1.2
122	0.0	0.0	0.1
123	0.9	1.1	0.9
125	0.0	0.0	0.0
126	0.1	0.2	0.2
127	0.0	0.0	0.1
129	0.0	0.0	0.0
132	5.5	4.8	2.8
134	0.2	0.5	3.6
136	0.1	0.2	0.4
144	0.0	0.0	0.0
149	0.0	0.0	0.0
155	0.0	0.1	2.0
157	0.0	0.0	0.0
160	25.1	31.5	34.2
162	0.0	0.0	0.0
163	0.0	0.0	0.0
167	0.0	0.1	0.1
170	0.0	0.0	0.1
175	0.7	1.0	0.7
179	0.0	0.0	0.0
182	7.3	5.3	2.5
184	0.0	0.0	0.1
189	0.0	0.0	0.2
192	0.0	0.0	0.2
195	0.0	0.0	0.0
199	0.0	0.0	0.1
1	7.6	5.6	2.7
201	0.0	0.0	0.1

202	0.0	0.0	0.1
203	0.0	0.0	0.1
206	0.2	0.5	2.8
211	0.0	0.0	0.1
212	0.0	0.0	0.0
215	0.0	0.0	0.1
220	0.0	0.0	0.0
221	0.0	0.0	0.1
224	0.0	0.0	0.0
225	0.0	0.0	0.1
24	5.3	4.0	0.5
34	0.2	0.5	2.6
41	0.1	0.2	0.1
48	0.2	0.5	3.4
58	0.0	0.0	0.0
63	0.1	0.2	0.2
65	0.3	0.2	0.1
87	0.2	0.5	1.7
97	0.0	0.0	0.0
176	0.0	0.0	0.0

- a. Percentage based on the relative bottom-of-the-well electronic energy.
- b. Percentage based on the relative ZPVE corrected electronic energy (see methods section).
- c. Percentage based on the relative 298 K free energy electronic energy.