

Carbohydrate Hydration: Heavy Water Complexes of Glucose, Galactose, Fucose and Xylose

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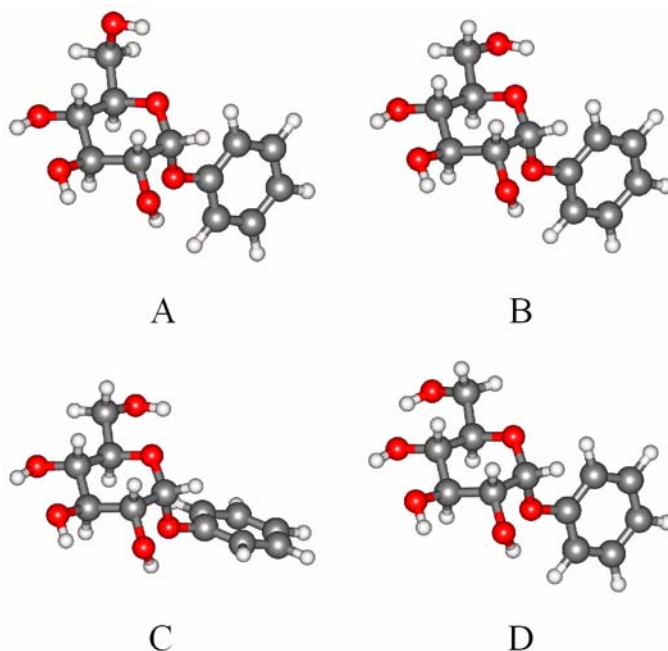
Supplementary information

The calculated relative energies, Cartesian coordinates of optimized geometries, and the vibrational frequencies of molecules of interest and their various lowest energy conformers, obtained using the Gaussian 03 package of programs, and derived at the B3LYP/6-31+G(d) level of theory are given in this supplementary information. More accurate single point energies were calculated for the optimised DFT structures, at the MP2/6-311++G(d,p) level of theory. All energies were corrected for zero point energy (ZPE) using the unscaled DFT harmonic frequencies. Provided information enable complete and precise reproduction of the calculated structures. In tables with coordinates of optimized geometries, the first column represents atomic number, followed by columns with *x*, *y* and *z* coordinates respectively. When present, coordinates of D₂O molecules are given at the bottom of the table. The origin of the coordinate system is the centre-of-mass of the molecular system. The geometrical coordinates are taken from the ‘Standard orientation’ table of the output file for each calculation.

Table 1. α -PhGlc

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6- 31+G(d) energy / kJ mol ⁻¹
A	0.00	0.00
B	0.94	1.69
C	3.52	2.23
D	0.14	2.80



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.023635	-0.364459	-0.937123
6	1.150103	-1.408524	-0.969449
6	2.044525	-1.274262	0.265478
6	2.545697	0.159108	0.413372
6	1.358115	1.127773	0.438683
8	0.531598	0.931025	-0.735303
8	0.645616	-2.733416	-1.103207
8	3.190265	-2.118350	0.167239
8	3.256168	0.332589	1.635283
6	1.765165	2.598489	0.409479
8	2.460245	2.951742	-0.779851
1	-0.093080	-2.824320	-0.475633
1	2.881968	-3.019585	-0.026509
1	1.875800	2.752977	-1.529328
1	-0.511419	-0.328463	-1.891542
1	1.753358	-1.227446	-1.864844
1	1.466996	-1.536928	1.165251
1	3.192367	0.404580	-0.440991
1	0.760796	0.941792	1.341418
1	3.960102	-0.336523	1.660141
1	0.864987	3.217990	0.534921
1	2.446227	2.796410	1.240199
8	-0.868808	-0.781255	0.091255
6	-3.069723	-1.018385	0.900159
6	-2.166377	-0.297223	0.111203
6	-2.582529	0.843253	-0.582958
6	-3.922155	1.240213	-0.496911
6	-4.833759	0.525364	0.281278
6	-4.398154	-0.603824	0.983992
1	-2.719348	-1.895792	1.436321
1	-1.876373	1.429328	-1.159360
1	-4.244670	2.125834	-1.038480
1	-5.869981	0.845160	0.345013
1	-5.095658	-1.168826	1.596876

B			
6	0.148497	-0.529502	-0.962020
6	1.360798	-1.470909	-0.880276
6	2.274849	-1.082784	0.285916
6	2.642285	0.397171	0.211770
6	1.361988	1.237362	0.169686
8	0.549058	0.818341	-0.955699
8	0.973049	-2.838173	-0.799768
8	3.492295	-1.824914	0.257867
8	3.399778	0.802247	1.345177
6	1.621200	2.724199	-0.035365
8	0.420330	3.483874	-0.004970
1	0.254553	-2.895959	-0.145274
1	3.266417	-2.768967	0.206654
1	-0.178849	3.114167	-0.673346
1	-0.395931	-0.675426	-1.900143
1	1.923726	-1.375402	-1.814411
1	1.751675	-1.263689	1.237535
1	3.218909	0.569961	-0.711443
1	0.792757	1.094954	1.096523
1	4.127105	0.166017	1.450498
1	2.246922	3.094525	0.779264
1	2.157816	2.872454	-0.985582
8	-0.689857	-0.869768	0.135723
6	-2.573270	0.415777	-0.783503
6	-2.020307	-0.484776	0.132221
6	-2.814702	-1.057803	1.131694
6	-4.168913	-0.736580	1.207992
6	-4.739554	0.152218	0.289852
6	-3.936823	0.721324	-0.699268
1	-1.959281	0.890651	-1.540047
1	-2.359385	-1.747903	1.836261
1	-4.780334	-1.185260	1.986550
1	-5.795182	0.401137	0.350247
1	-4.364435	1.421699	-1.412121

C			
6	-0.102310	-0.683519	0.792376
6	-1.319670	-1.607574	0.624152
6	-2.308515	-1.032882	-0.394638
6	-2.663482	0.411254	-0.049854
6	-1.376074	1.234855	0.036226
8	-0.493319	0.646520	1.021210
8	-0.934632	-2.933120	0.274741
8	-3.525098	-1.777358	-0.412445
8	-3.496969	0.993248	-1.044680
6	-1.592270	2.673898	0.486000
8	-0.369787	3.400486	0.518372
1	-0.265889	-2.855972	-0.429413
1	-3.301310	-2.713471	-0.548210
1	0.237430	2.919567	1.104726
1	0.494357	-0.964687	1.665649
1	-1.821961	-1.687911	1.593675
1	-1.850716	-1.047427	-1.395900
1	-3.171793	0.427556	0.927794
1	-0.877327	1.235591	-0.940957
1	-4.229288	0.374905	-1.206526
1	-2.242933	3.182894	-0.227987
1	-2.080158	2.680425	1.473051
8	0.684875	-0.835753	-0.390839
6	2.422276	0.777122	-0.819052
6	2.024036	-0.456762	-0.302980
6	2.955493	-1.338444	0.250723
6	4.303864	-0.973337	0.292572
6	4.715807	0.260486	-0.220367
6	3.773851	1.131238	-0.776359
1	1.680810	1.445177	-1.245829
1	2.624882	-2.300426	0.633622
1	5.032133	-1.657815	0.719766
1	5.765379	0.540085	-0.189674
1	4.087782	2.091308	-1.177438

D			
6	-0.043267	-0.630560	-0.960493
6	1.071030	-1.675949	-0.785351
6	2.055534	-1.242254	0.306143
6	2.549914	0.171039	0.026043
6	1.356723	1.129464	-0.081797
8	0.484840	0.661785	-1.132619
8	0.553091	-2.975598	-0.525753
8	3.199782	-2.093020	0.343988
8	3.414878	0.640491	1.061844
6	1.763321	2.560732	-0.448260
8	2.365329	3.239493	0.642224
1	-0.155124	-2.875487	0.134858
1	2.889403	-3.010934	0.420945
1	3.075528	2.672457	0.991811
1	-0.634039	-0.829964	-1.860145
1	1.612496	-1.753739	-1.733739
1	1.551298	-1.254144	1.284373
1	3.090956	0.171304	-0.933413
1	0.811157	1.153138	0.870203
1	4.093710	-0.039356	1.211260
1	2.425760	2.543357	-1.328496
1	0.864712	3.125281	-0.712510
8	-0.873032	-0.751625	0.189998
6	-3.028351	-0.746701	1.144781
6	-2.167229	-0.256762	0.156714
6	-2.615787	0.684137	-0.775387
6	-3.947459	1.112100	-0.720482
6	-4.818030	0.625800	0.255924
6	-4.349024	-0.302541	1.192171
1	-2.652158	-1.469916	1.862838
1	-1.939462	1.099733	-1.513405
1	-4.295486	1.843211	-1.445673
1	-5.848030	0.969099	0.292637
1	-5.014083	-0.687282	1.960967

(d) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	31.7059	0.2307	29.5334	0.3291	24.9334	0.1552
v2	46.0997	0.0819	45.8154	0.0548	35.6305	0.4789
v3	52.3912	0.5382	52.0861	0.1106	47.5285	0.1342
v4	95.9313	1.5629	93.9109	2.9786	92.8769	1.2128
v5	98.7639	1.7867	113.0738	0.1349	102.3917	2.1191
v6	116.8840	2.3875	117.7719	1.3083	120.2695	1.4852
v7	141.7400	1.7170	138.9700	1.3320	125.2440	0.5369
v8	194.0669	2.7029	183.1888	0.5909	178.1919	1.2226
v9	204.9277	5.1638	199.5240	1.0588	197.6618	2.7955
v10	238.7902	10.8748	237.5383	8.6319	233.3316	8.9991
v11	253.6405	12.0944	250.9722	8.6300	249.2919	2.8121
v12	262.1043	5.9580	260.1357	9.6434	257.1790	15.2676
v13	282.5573	11.1176	294.0583	2.4768	312.7009	7.5430
v14	315.8760	12.3535	327.3364	32.1313	348.5426	14.6741
v15	348.6944	1.4346	363.9630	3.9633	374.5588	11.3484
v16	370.1149	121.0732	381.0581	63.0385	386.7843	66.8334
v17	379.2492	38.0305	388.6704	69.4670	393.9841	25.9287
v18	399.2681	119.2434	402.5706	188.4744	414.8505	182.6943
v19	419.4580	31.5156	410.4524	15.6777	416.1705	13.3343
v20	422.5302	0.0607	422.8435	3.4934	424.5602	2.2791
v21	451.8929	23.0624	426.9244	5.7661	432.9816	92.1023
v22	473.2757	174.9953	456.5325	1.0305	450.6884	6.8202
v23	504.1992	6.2255	477.9257	177.6609	488.9609	113.5877
v24	516.3315	21.4959	517.3210	8.5141	505.5165	42.0204
v25	529.9412	19.2957	534.5626	14.3978	538.0057	33.1088
v26	538.6493	4.1132	554.6938	2.3527	559.1709	2.9470
v27	571.2267	16.7044	580.1014	12.1003	579.3548	10.7853
v28	622.2886	0.9971	602.9297	21.9803	604.2473	28.3691
v29	640.0217	7.1990	628.7158	2.3690	628.7655	0.6675
v30	699.1062	25.4497	676.4426	15.9008	664.5018	14.9429
v31	707.0185	18.9822	699.6522	19.6466	706.4457	36.5021
v32	751.5893	0.9138	744.3258	3.2145	740.7215	11.0205
v33	765.5214	70.7442	764.5990	70.6087	779.7742	28.6380
v34	836.2263	0.1217	829.9995	8.5572	837.1183	20.7487
v35	852.1220	25.0415	836.2813	4.3862	847.3828	1.1269
v36	881.1514	42.6186	866.9684	80.2918	869.8719	69.5062
v37	906.8253	10.4443	905.2232	8.1108	908.2703	47.6505
v38	918.2851	20.3977	930.9255	32.4401	936.2965	17.2171
v39	932.1267	43.9702	970.9491	0.4125	977.8930	0.3904
v40	971.5982	0.3506	993.9244	0.0992	996.5854	46.9896
v41	993.6806	0.1049	1001.0912	12.5411	1000.5882	3.1899
v42	1006.4591	142.4995	1013.4312	27.3896	1009.4348	127.8613
v43	1015.0830	9.0290	1021.2482	141.7640	1021.4757	38.5884
v44	1020.3306	71.2843	1033.0010	86.1158	1035.1554	66.8501
v45	1041.7975	138.5951	1053.8975	20.6984	1048.2650	14.1337
v46	1054.0325	69.2420	1062.5019	48.2268	1060.2921	38.6359
v47	1070.6028	73.0007	1071.7378	196.8865	1069.7714	148.9580
v48	1096.1466	247.5946	1095.2692	201.6560	1095.0514	229.2426
v49	1101.6850	93.9109	1098.2982	69.2553	1098.1202	21.2146
v50	1109.5023	38.1410	1111.6119	13.9089	1103.6831	11.5359
v51	1111.3468	55.4777	1114.6354	116.2338	1114.7638	135.2648
v52	1128.7105	18.6572	1133.5798	65.6505	1135.0667	62.6927
v53	1137.8238	56.7514	1145.6695	12.9400	1144.1765	19.6323
v54	1155.9508	55.3158	1153.4295	48.3143	1152.9365	48.0853
v55	1188.6757	3.0009	1188.8887	3.4627	1189.3521	0.0762
v56	1205.3644	15.3664	1207.8434	16.1082	1196.0860	12.7358
v57	1213.3468	17.2808	1214.4605	11.9085	1214.2093	8.5278
v58	1239.7487	24.4908	1231.8786	23.2218	1234.9168	14.2159
v59	1250.8591	279.8106	1250.0373	285.6456	1239.3565	197.6040
v60	1256.8481	27.8936	1259.1329	25.5394	1259.2015	10.8671
v61	1263.3923	44.5753	1266.3648	45.1350	1266.8005	55.9131
v62	1311.1343	6.4430	1309.8141	6.4478	1312.2934	8.4701
v63	1335.9826	63.4438	1329.3033	49.8343	1329.2228	57.2146
v64	1346.0351	5.4128	1347.4798	2.6029	1334.4590	0.5818
v65	1350.5800	0.4351	1353.4851	6.1386	1356.1228	1.4817
v66	1364.9609	7.3656	1361.0551	22.2140	1359.5320	12.7698
v67	1368.0829	7.6093	1367.8480	5.0336	1360.6062	18.5143
v68	1373.7768	21.9029	1380.7353	30.6707	1372.1410	20.9123
v69	1389.3247	7.4770	1391.5180	7.4719	1393.9976	9.0020
v70	1396.0782	31.1480	1398.8741	11.5371	1400.5493	10.8638
v71	1416.2921	2.8193	1413.0520	16.9409	1410.9243	9.5301
v72	1430.5856	34.6008	1434.7458	12.6670	1434.2157	19.6734
v73	1435.7283	16.0339	1435.1315	15.5888	1438.6028	15.1994
v74	1442.8097	19.7372	1442.7899	23.6244	1444.4717	20.2712
v75	1454.8492	9.1521	1455.8674	15.8917	1455.6977	13.0643

v76	1498.5493	0.6799	1498.9197	0.6974	1492.7389	1.3833
v77	1515.2200	7.5272	1517.0480	2.2531	1517.6514	1.9591
v78	1536.0360	97.7085	1537.2513	97.1541	1534.6041	70.1290
v79	1640.0267	23.6732	1641.2396	25.3600	1641.5225	6.9246
v80	1652.1962	60.2304	1652.8315	61.0438	1646.4411	39.8283
v81	3015.0180	16.8191	2999.9541	6.7151	3000.8991	7.6462
v82	3025.1557	45.2213	3012.5049	41.5989	3015.7451	34.4322
v83	3040.9749	5.5907	3019.3845	46.4214	3019.2746	47.8619
v84	3058.9287	46.9808	3073.7755	23.9086	3067.7560	30.8764
v85	3091.1366	14.3947	3093.2390	12.9685	3092.8207	12.7644
v86	3102.2043	25.5873	3102.6872	28.1651	3102.6604	27.0226
v87	3142.8141	8.6024	3146.0223	8.6637	3146.3367	9.6509
v88	3185.6587	1.5047	3186.1331	1.7907	3184.8591	1.4989
v99	3193.2407	10.2980	3193.5275	9.4775	3193.3251	5.9517
v90	3205.2237	23.1413	3205.6189	22.1346	3201.8497	21.0248
v91	3213.1951	13.9241	3213.6274	14.9688	3210.5628	18.1405
v92	3234.4106	1.4631	3231.3671	3.8300	3221.5823	2.4170
v93	3707.3619	47.4111	3706.4059	48.6969	3696.5326	50.4683
v94	3728.5943	42.9263	3728.4083	37.6733	3728.8591	25.2660
v95	3738.3304	57.4392	3730.4857	64.8972	3729.7225	77.5189
v96	3742.6545	22.5390	3745.6607	25.8610	3735.2649	26.6471

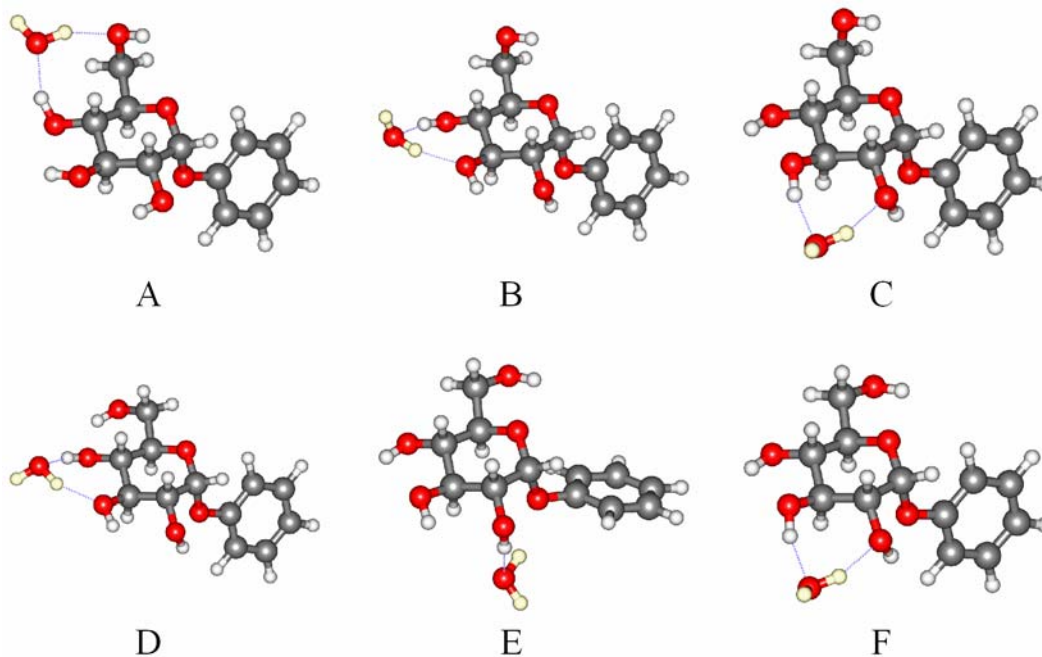
D		
	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	28.4502	0.4658
v2	40.7916	0.1084
v3	51.7642	0.7029
v4	88.8692	0.6436
v5	104.7656	1.2706
v6	134.5809	0.3676
v7	152.7423	6.3879
v8	190.8709	4.2606
v9	201.8512	2.3672
v10	233.8627	10.3227
v11	259.3395	2.7320
v12	270.7045	6.5445
v13	293.1419	5.2176
v14	338.7710	1.3015
v15	348.7269	10.2590
v16	379.8566	79.7328
v17	402.4735	64.8414
v18	411.0599	8.2993
v19	422.1921	1.7294
v20	426.5751	9.3943
v21	471.8274	176.6736
v22	487.7719	11.7463
v23	508.6204	115.5625
v24	512.9443	40.5690
v25	519.4320	18.8903
v26	535.1633	28.0375
v27	574.3518	10.8352
v28	588.7739	3.6941
v29	627.7114	0.9215
v30	669.4165	15.8296
v31	700.7793	21.7246
v32	737.2138	5.2309
v33	766.3917	68.8640
v34	837.5148	0.0463
v35	860.1427	42.9285
v36	897.6322	12.9441
v37	908.8359	14.8567
v38	927.3423	41.9476
v39	972.3441	0.3970
v40	981.0212	65.1676
v41	994.2915	0.1101
v42	1009.8239	32.3816
v43	1014.2345	22.2097
v44	1027.3320	172.7091
v45	1052.5519	27.3387
v46	1065.4837	103.7197
v47	1086.9623	47.8558
v48	1095.2700	366.7426
v49	1107.1850	33.8998
v50	1109.8157	7.5548
v51	1114.2060	76.6057
v52	1132.6895	82.4034
v53	1148.5215	37.9254
v54	1151.8491	27.4969
v55	1188.6061	2.8384
v56	1193.1706	4.7386
v57	1204.8824	19.6912
v58	1238.1330	39.6752
v59	1250.4853	267.0804
v60	1264.7301	50.6558
v61	1277.5779	33.9439
v62	1310.0138	9.8079
v63	1326.1686	13.8139
v64	1344.6206	6.3675
v65	1350.5746	24.5495
v66	1364.0128	15.0497
v67	1365.9262	3.5531
v68	1376.3285	22.0708
v69	1395.2308	0.7836
v70	1398.7093	28.0311
v71	1415.0822	4.4137
v72	1440.4346	23.7727
v73	1444.8962	9.1116
v74	1446.4277	4.0889
v75	1455.7379	84.2895

v76	1498.7860	0.7072
v77	1527.6387	1.6941
v78	1535.7251	97.8249
v79	1640.1718	23.5579
v80	1652.1993	59.2004
v81	3001.6472	22.9219
v82	3008.4666	32.5953
v83	3024.6557	35.5409
v84	3065.4489	28.4959
v85	3093.2460	12.5332
v86	3102.5621	27.3267
v87	3116.8811	25.8693
v88	3185.6294	1.5441
v99	3193.2068	9.7914
v90	3204.5781	23.1441
v91	3212.8765	14.7989
v92	3233.5162	0.9000
v93	3698.5890	108.4098
v94	3704.5768	54.9713
v95	3729.5548	31.8317
v96	3730.7606	61.8953

Table 2. α -PhGlc $\cdot$ D₂O

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	0.02	0.00
B	1.76	6.25
C	1.14	6.90
D	0.14	7.57
E	12.02	7.78
F	1.33	8.00



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.431964	0.554960	-0.924336
6	-0.573010	1.714752	-0.934901
6	-1.493827	1.638685	0.281480
6	-2.175487	0.271968	0.328329
6	-1.090849	-0.822019	0.342154
8	-0.266433	-0.682421	-0.837978
8	0.128347	2.941926	-1.013804
8	-2.441773	2.695382	0.145408
8	-3.004575	0.225914	1.482344
6	-1.614877	-2.249505	0.329126
8	-2.494385	-2.524407	-0.772836
1	-0.526440	3.650470	-0.894757
1	-3.095753	2.584403	0.856474
1	-2.033987	-2.284150	-1.594339
1	0.988209	0.511582	-1.865799
1	-1.192925	1.577891	-1.835283
1	-0.905966	1.783521	1.199179
1	-2.787195	0.160907	-0.576701
1	-0.469840	-0.704179	1.240822
1	-3.797932	-0.303871	1.253400
1	-0.767381	-2.946041	0.309111
1	-2.198502	-2.433772	1.233949
8	1.315943	0.738561	0.155993
6	2.845803	-1.011514	-0.635285
6	2.544221	0.109821	0.145904
6	3.506515	0.654862	1.004718
6	4.774707	0.081256	1.075235
6	5.095163	-1.032280	0.289348
6	4.127984	-1.569111	-0.561482
1	2.092323	-1.460180	-1.272661
1	3.244994	1.528134	1.594730
1	5.518609	0.511609	1.740939
1	6.085766	-1.475323	0.343075
1	4.360711	-2.438964	-1.170878
8	-4.865398	-1.433477	0.193383
1	-5.560856	-2.044706	0.475595
1	-4.197487	-1.960399	-0.298669

B			
6	0.389726	-0.252754	1.022013
6	-0.809976	-1.195004	1.165153
6	-1.761752	-1.064809	-0.027172
6	-2.165854	0.394182	-0.266642
6	-0.907875	1.277008	-0.339868
8	-0.037448	1.065300	0.799559
8	-0.412424	-2.551387	1.352813
8	-2.935853	-1.852880	0.234809
8	-2.832757	0.572455	-1.502657
6	-1.224304	2.770161	-0.331316
8	-1.843268	3.190483	0.879742
1	0.279864	-2.741499	0.695009
1	-2.633982	-2.736539	0.508466
1	-1.236708	2.973367	1.606204
1	0.984772	-0.224603	1.940790
1	-1.347445	-0.915169	2.076983
1	-1.274433	-1.440183	-0.937863
1	-2.791173	0.732784	0.572890
1	-0.363412	1.034679	-1.262132
1	-3.746425	0.217210	-1.435597
1	-0.295311	3.331448	-0.508769
1	-1.928296	2.988897	-1.136474
8	1.180087	-0.779153	-0.038722
6	3.050646	0.731279	0.460232
6	2.506776	-0.399415	-0.157533
6	3.301615	-1.219811	-0.965919
6	4.650093	-0.914927	-1.145536
6	5.213183	0.203171	-0.519821
6	4.408747	1.017792	0.278136
1	2.428596	1.393514	1.051271
1	2.852430	-2.086630	-1.442277
1	5.263126	-1.556518	-1.773165
1	6.264773	0.437695	-0.658599
1	4.830806	1.896018	0.760016
8	-5.206035	-0.830793	-1.002769
1	-5.879565	-0.493139	-0.394295
1	-4.612183	-1.404778	-0.475026

C			
6	-0.103175	-0.095766	-0.928698
6	1.213574	-0.893986	-0.928031
6	2.081367	-0.536615	0.289209
6	2.223273	0.983622	0.410583
6	0.855248	1.666201	0.425895
8	0.109886	1.278011	-0.755578
8	0.920228	-2.296803	-1.011207
8	3.404900	-1.042004	0.189280
8	2.889796	1.324771	1.619542
6	0.923207	3.190474	0.385183
8	1.529752	3.683024	-0.802919
1	0.182378	-2.461801	-0.396095
1	3.403401	-2.020805	0.277455
1	1.013403	3.349416	-1.554415
1	-0.623450	-0.200234	-1.886512
1	1.765915	-0.649385	-1.840168
1	1.595487	-0.915727	1.201683
1	2.795208	1.351952	-0.453573
1	0.301851	1.360234	1.323842
1	3.696898	0.782850	1.652908
1	-0.093601	3.594124	0.500801
1	1.536833	3.540995	1.218128
8	-0.900434	-0.670478	0.105852
6	-2.915568	0.525076	-0.633000
6	-2.270453	-0.464832	0.114853
6	-3.002657	-1.315487	0.950851
6	-4.388278	-1.183311	1.028318
6	-5.050389	-0.208817	0.272987
6	-4.308598	0.637844	-0.551836
1	-2.348753	1.214808	-1.247254
1	-2.476370	-2.068831	1.530226
1	-4.951861	-1.847247	1.678613
1	-6.130437	-0.108739	0.332558
1	-4.809151	1.406969	-1.134475
8	3.010689	-3.815196	0.014995
1	3.615396	-4.318446	-0.550018
1	2.263013	-3.527155	-0.551311

D			
6	-0.427899	-0.580478	-1.018132
6	0.766711	-1.535612	-0.904680
6	1.766861	-1.059729	0.155989
6	2.160697	0.396859	-0.103176
6	0.883528	1.253961	-0.171873
8	0.003974	0.742976	-1.195840
8	0.368463	-2.880905	-0.654071
8	2.925925	-1.907718	0.108666
8	2.977866	0.942293	0.925968
6	1.165886	2.718497	-0.526686
8	1.743433	3.426379	0.556861
1	-0.315132	-2.853360	0.039014
1	2.605037	-2.825681	0.062704
1	2.473954	2.876811	0.897864
1	-1.039581	-0.815713	-1.895076
1	1.272290	-1.552766	-1.875702
1	1.316292	-1.126140	1.156343
1	2.679629	0.458076	-1.072818
1	0.372995	1.223955	0.799247
1	3.884571	0.562269	0.856119
1	1.803287	2.764733	-1.424785
1	0.217403	3.210736	-0.760891
8	-1.197860	-0.775472	0.163934
6	-3.067325	0.553015	-0.713558
6	-2.519052	-0.357345	0.195279
6	-3.300622	-0.895154	1.223716
6	-4.641396	-0.529532	1.335396
6	-5.209350	0.367467	0.423653
6	-4.417582	0.901991	-0.593657
1	-2.453296	1.006526	-1.482954
1	-2.847872	-1.592987	1.922408
1	-5.244437	-0.950623	2.135642
1	-6.254657	0.649995	0.511024
1	-4.842773	1.610101	-1.300294
8	5.292479	-0.546150	0.573828
1	4.671197	-1.291111	0.431818
1	5.824119	-0.769682	1.351963

E			
6	0.114427	-0.360068	-0.968634
6	1.361026	-1.264439	-0.978114
6	2.352090	-0.847302	0.115756
6	2.664400	0.643889	0.011648
6	1.359976	1.443771	0.054931
8	0.481335	0.995938	-1.005235
8	1.069338	-2.648965	-0.940048
8	3.588008	-1.546688	-0.018445
8	3.485877	1.082903	1.087620
6	1.546997	2.938593	-0.168588
8	0.311624	3.639907	-0.084548
1	0.680309	-2.884163	-0.068261
1	3.383505	-2.492796	-0.111796
1	-0.288450	3.247433	-0.739971
1	-0.489911	-0.525447	-1.864822
1	1.842788	-1.097331	-1.948416
1	1.923579	-1.047852	1.109472
1	3.170871	0.826646	-0.949914
1	0.865696	1.286559	1.021837
1	4.235607	0.467334	1.149195
1	2.028001	3.106560	-1.144547
1	2.193336	3.343225	0.612841
8	-0.685217	-0.659607	0.188792
6	-2.925922	-1.049289	-0.622939
6	-2.027513	-0.279555	0.120920
6	-2.460513	0.829834	0.847989
6	-3.815970	1.171731	0.827255
6	-4.725260	0.414331	0.082841
6	-4.277582	-0.694672	-0.641908
1	-2.565992	-1.915735	-1.171721
1	-1.742732	1.413712	1.415765
1	-4.157932	2.035404	1.391344
1	-5.777329	0.685592	0.068609
1	-4.980487	-1.290596	-1.218204
8	-0.017797	-2.990966	1.646961
1	-0.678606	-3.656418	1.890312
1	-0.504532	-2.163256	1.470570

F			
6	0.002779	-0.189427	-0.985778
6	1.397733	-0.843352	-0.934726
6	2.247196	-0.271780	0.212455
6	2.221845	1.259027	0.172390
6	0.782526	1.772401	0.191263
8	0.070499	1.209165	-0.941541
8	1.252782	-2.269358	-0.861859
8	3.615586	-0.639462	0.121670
8	2.909411	1.802204	1.290046
6	0.674302	3.283656	0.040338
8	-0.673031	3.732036	0.111691
1	0.533224	-2.440999	-0.226853
1	3.722865	-1.597988	0.312865
1	-1.178781	3.251952	-0.563651
1	-0.504571	-0.437128	-1.923616
1	1.906986	-0.642021	-1.881903
1	1.824769	-0.600871	1.174374
1	2.704926	1.585535	-0.763495
1	0.282993	1.464326	1.117966
1	3.749769	1.316179	1.359613
1	1.209282	3.764285	0.861898
1	1.141823	3.589133	-0.908802
8	-0.722036	-0.747873	0.108171
6	-2.729203	-1.476544	1.099116
6	-2.106608	-0.695750	0.118811
6	-2.868528	0.075028	-0.764502
6	-4.264679	0.039279	-0.667808
6	-4.896813	-0.739596	0.301982
6	-4.120093	-1.494423	1.188231
1	-2.114094	-2.057460	1.780492
1	-2.394252	0.709662	-1.504162
1	-4.855572	0.639081	-1.355245
1	-5.980674	-0.754977	0.372310
1	-4.597717	-2.102593	1.951946
8	3.503009	-3.430566	0.282390
1	2.717533	-3.294306	-0.289765
1	4.138996	-3.952084	-0.229151

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	26.5694	0.2832	26.8824	1.0245	26.0412	0.4364
v2	42.1514	0.0565	31.7853	0.3521	38.8545	1.7433
v3	45.7646	0.1319	43.8510	0.0897	40.4138	0.1535
v4	55.4459	1.4621	54.8076	2.3848	45.9941	0.4061
v5	95.3385	1.5868	87.4551	4.0541	88.9870	0.3752
v6	102.6379	2.0325	93.9340	0.9570	98.0557	4.3541
v7	115.2732	4.8049	117.6346	1.2335	112.8805	1.1280
v8	141.3157	10.7245	137.0062	5.4177	137.7839	0.3901
v9	153.8988	49.0338	153.4015	9.2106	143.6222	12.3908
v10	181.8989	28.1267	172.0402	1.5674	158.4528	1.6617
v11	191.7545	6.5960	193.7736	14.5359	200.8143	60.8942
v12	211.9496	7.4916	203.2870	70.6759	209.8429	15.1629
v13	221.1866	17.9120	209.3259	6.3251	224.4451	48.1297
v14	249.0135	8.4917	235.7055	25.2135	254.8941	12.5093
v15	265.5815	9.4193	261.6119	7.1560	256.9385	34.8717
v16	266.9622	7.7111	279.0544	6.7545	275.6236	36.4728
v17	283.0768	29.8447	290.5014	1.9859	298.6549	17.4307
v18	313.0528	40.3567	309.1776	1.2945	321.9639	20.9245
v19	331.9871	28.3739	326.2064	5.2746	334.5185	21.5470
v20	355.4246	12.8008	354.5184	7.8807	350.8133	2.5374
v21	380.6129	93.9734	400.4014	57.7342	389.5084	101.6568
v22	396.5321	102.3288	407.4666	86.4782	414.4506	51.7164
v23	415.0590	17.6525	418.9167	43.2783	422.4329	26.1608
v24	421.9045	77.4465	423.5022	0.1038	423.5181	99.4332
v25	424.3469	1.0923	448.5935	19.4833	455.3439	29.6525
v26	446.9921	41.2659	485.3398	6.9759	461.1983	33.2634
v27	505.2949	0.9428	499.0038	158.1881	507.3031	12.1421
v28	518.1568	20.2455	512.2749	30.9224	516.7938	7.2500
v29	525.8501	18.6289	527.3496	124.4883	528.0865	43.3247
v30	537.2087	12.9442	532.4658	32.3355	537.7923	9.9081
v31	543.0983	19.2244	540.2311	36.7515	553.7449	72.2736
v32	570.1581	24.3914	573.2263	29.8477	567.9905	12.3208
v33	621.2800	5.0977	622.3128	0.6346	623.0116	1.1410
v34	638.5519	16.2064	640.4843	6.2096	640.6153	7.6844
v35	700.0018	14.3495	700.0979	24.0565	698.8619	24.8251
v36	709.5330	79.8745	707.1988	17.0806	706.1519	17.9711
v37	719.0737	66.9195	750.5234	21.7606	751.2664	10.4884
v38	750.4852	5.3906	761.3548	81.7657	759.8848	100.1798
v39	765.5831	64.2901	765.7647	71.9530	765.5173	65.9558
v40	839.4765	0.7599	837.7687	0.1431	834.8303	0.2192
v41	846.7510	20.5399	852.7032	27.8299	849.9183	19.4677
v42	867.8947	35.2176	880.0527	42.6990	881.9106	42.3170
v43	907.3680	7.8741	908.6608	12.2874	906.2751	10.2834
v44	924.2858	5.5782	923.2227	19.5608	922.4588	16.5739
v45	937.1739	34.8382	933.0132	41.8913	930.3971	52.0011
v46	971.7196	0.3437	972.3558	0.3384	971.2637	0.3073
v47	991.7156	0.0905	993.8384	0.1254	993.9601	0.0776
v48	1013.2228	38.7392	1003.4977	110.1859	1007.5645	124.1408
v49	1017.9780	55.7484	1014.8610	0.4680	1015.1438	10.7299
v50	1031.2470	381.0930	1024.1307	86.4577	1023.6277	115.5905
v51	1035.9995	121.9067	1041.5442	143.7727	1044.2959	121.0964
v52	1052.1985	42.6044	1053.3873	64.0559	1053.7514	62.8584
v53	1063.6342	155.0073	1070.0996	100.5729	1065.3469	110.1842
v54	1098.3081	9.8381	1097.4858	243.3924	1097.7822	140.6804
v55	1107.4617	2.4352	1102.6444	124.3116	1108.3428	59.2445
v56	1113.6101	38.3828	1108.1849	45.9770	1110.0128	14.6815
v57	1121.1358	72.3657	1110.1206	5.7671	1113.8381	116.1820
v58	1132.3583	86.3907	1127.4138	17.3503	1131.6933	58.9099
v59	1145.5135	47.0882	1137.2106	73.7561	1137.2742	45.8428
v60	1151.8336	34.8165	1158.3258	41.1539	1145.8146	91.0023
v61	1187.3692	2.8090	1188.5782	3.1891	1188.7711	3.0555
v62	1202.7956	19.5559	1205.1936	15.3663	1204.9865	20.6454
v63	1221.1826	47.0544	1218.2491	9.7695	1218.3123	48.8612
v64	1227.3460	38.5734	1229.5246	26.1913	1226.1944	14.8514
v65	1235.4235	37.5703	1240.4848	32.7086	1241.6573	72.5472
v66	1260.7151	261.6980	1251.3064	278.1093	1251.5731	203.9212
v67	1265.7274	31.6403	1258.6177	32.6722	1260.8921	33.1892
v68	1271.6061	23.4422	1286.3584	59.3465	1285.1493	63.1691
v69	1316.3424	32.2907	1313.7563	4.5258	1305.0207	1.5156
v70	1341.9943	2.9513	1344.0079	21.5514	1345.3982	4.4524
v71	1350.0507	13.0722	1347.3160	34.6271	1346.2639	4.2646
v72	1363.1563	9.5730	1362.2857	19.1069	1351.2806	20.6871
v73	1366.7143	13.7931	1367.5933	9.5999	1366.1028	3.3167
v74	1368.0634	6.0779	1369.5741	9.2851	1378.1891	44.6357
v75	1381.6310	20.8172	1375.3655	16.4915	1387.7131	11.5411

v76	1400.7994	26.6302	1396.0366	35.4431	1395.7026	47.1089
v77	1410.3333	49.7955	1410.8468	10.0617	1398.5553	20.6573
v78	1426.3082	4.7275	1413.0359	2.8844	1413.9421	1.4951
v79	1433.7330	25.8246	1428.8621	32.5374	1432.2196	33.5822
v80	1443.2922	26.2022	1432.3444	8.7206	1442.4855	31.3428
v81	1448.8791	16.8313	1442.4033	29.8701	1456.8964	12.8293
v82	1475.8000	18.4491	1474.4439	15.3895	1467.5106	23.3851
v83	1497.6976	0.4950	1498.4836	0.7472	1498.7428	0.6926
v84	1514.3440	7.9146	1515.3389	8.7370	1512.5436	7.9931
v85	1536.0534	103.9461	1536.0029	98.4768	1535.8614	97.9620
v86	1637.7450	22.1564	1639.9493	24.0197	1640.0132	24.7628
v87	1652.5304	69.8580	1652.1988	61.5500	1652.1685	60.6098
v88	2563.7229	177.4769	2599.8370	148.0273	2582.8701	171.4153
v89	2795.5523	86.0548	2792.7580	91.4042	2791.5501	100.8574
v90	3003.6073	24.1639	3024.9262	23.9134	3012.8074	12.4821
v91	3036.6106	7.0437	3027.8385	28.5971	3022.9575	50.1023
v92	3044.4363	6.6851	3043.4924	13.9994	3034.2840	10.3214
v93	3057.7460	22.5565	3061.3071	41.2840	3058.4419	44.1698
v94	3064.3447	65.0606	3088.6658	16.1545	3089.8305	18.2332
v95	3099.3073	22.3526	3100.9729	25.5067	3109.6945	19.3930
v96	3141.6385	12.4603	3150.0473	7.9056	3142.1349	8.2368
v97	3182.1790	1.4457	3185.6384	1.5675	3185.9306	1.5049
v98	3190.5756	16.1037	3193.1957	10.3848	3193.5163	9.9225
v99	3205.8830	29.1681	3205.2654	22.9901	3205.0577	22.3204
v100	3215.1734	6.9705	3213.1317	14.1777	3213.1840	14.1866
v101	3230.1111	2.7831	3233.7203	1.4689	3235.2299	1.6140
v102	3556.4392	507.4390	3524.2785	674.8251	3519.5239	615.3169
v103	3725.3753	48.4667	3705.4486	50.8110	3692.0287	78.5842
v104	3727.2916	58.1086	3714.5621	51.9094	3720.3995	55.6938
v105	3737.2970	39.5585	3742.1564	23.0239	3743.1877	22.8779

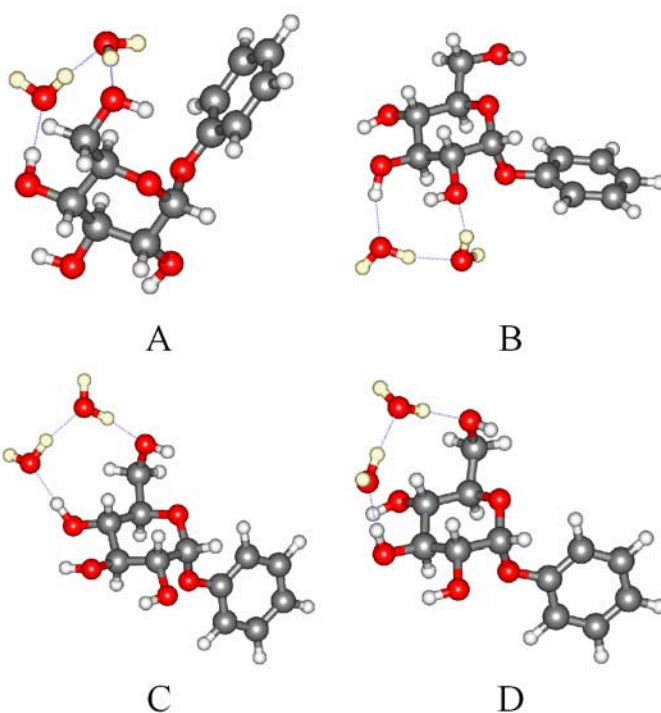
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	24.9004	1.4348	26.1006	0.1043	27.6917	0.6381
v2	30.6024	2.0881	33.7827	0.2780	39.1911	0.5294
v3	43.2807	0.3109	37.1466	0.6223	44.2415	0.6049
v4	58.9137	1.1324	54.3616	3.3042	47.5714	0.1152
v5	86.1285	1.4403	78.0536	2.2625	94.5756	3.0292
v6	98.7299	2.0306	95.9307	1.5288	105.3297	0.4123
v7	126.7415	1.6929	116.1189	2.3053	115.4353	3.0712
v8	148.5235	1.8935	122.3739	0.5489	133.0668	0.2595
v9	154.6365	7.0484	134.0328	16.7643	147.4790	13.9825
v10	174.2367	0.8596	146.9943	3.8286	160.1606	1.2586
v11	195.8368	6.4231	182.3192	48.6761	186.7287	0.2930
v12	203.6272	82.6086	192.8729	8.7247	203.0878	62.2684
v13	223.8806	7.2886	223.6846	31.5671	226.1875	53.3615
v14	258.3356	1.0078	230.6872	15.2578	246.6585	18.6273
v15	276.8242	40.2059	249.6975	4.3624	275.4841	71.5555
v16	277.7728	18.9447	255.5283	33.2600	278.3085	11.4152
v17	310.1998	5.3352	271.4059	32.1623	296.2027	2.7455
v18	328.9674	5.1228	318.3092	18.8223	331.3023	5.5060
v19	343.8960	5.0927	345.8338	20.1619	335.7713	23.4718
v20	372.8358	7.6422	370.1383	42.6643	371.3623	8.4829
v21	408.8675	59.6471	386.1394	59.9395	392.1703	89.7433
v22	411.2701	3.3448	388.4489	28.3580	407.5879	59.6304
v23	421.6539	1.7551	396.5073	11.5895	422.2464	2.2637
v24	424.4973	2.5871	413.4911	189.8660	428.0907	33.2033
v25	468.0461	62.3328	416.0052	50.4113	440.2538	139.4822
v26	489.7099	19.2465	425.8952	9.8741	464.6464	18.4224
v27	505.7383	170.6258	436.4998	37.7202	467.3308	29.9040
v28	516.6278	1.9643	452.6079	9.0569	517.3724	5.9303
v29	520.3480	36.8637	501.7847	12.4583	535.4562	18.4643
v30	539.1762	31.7756	533.3988	3.3854	545.6807	40.6579
v31	561.1784	66.7241	558.8554	2.6814	563.7193	36.1140
v32	579.4862	41.9942	584.2188	10.6955	578.7339	27.7770
v33	593.3283	18.3903	604.9363	23.9951	611.6828	11.2053
v34	627.8560	1.4333	628.4826	0.4242	628.6118	2.6852
v35	671.6762	16.2158	671.0496	16.9016	675.9791	14.8908
v36	700.3464	21.5717	708.4082	39.6747	700.6811	19.4149
v37	738.9366	8.0047	731.8709	9.5782	745.1171	2.6757
v38	766.2141	69.9451	756.1461	156.8549	764.6526	105.3645
v39	780.2820	138.0201	781.9008	39.5171	765.6268	71.3307
v40	836.7514	0.0647	836.7176	25.4767	829.5169	12.1385
v41	861.1078	50.4488	849.3318	1.1100	836.7573	3.6499
v42	905.7966	15.0550	868.2969	69.2106	867.3466	73.1721
v43	908.4845	13.4718	898.7757	88.2767	906.0061	8.9126
v44	929.2531	44.7306	938.6512	16.2610	929.9389	40.1745
v45	972.1001	0.3398	979.8275	0.4855	971.1183	0.4648
v46	986.1969	65.8616	994.1692	98.0823	994.0014	0.1129
v47	994.1874	0.1403	1002.3591	2.0088	1006.8732	14.9459
v48	1004.8697	17.8386	1010.3512	121.5994	1013.3643	37.4320
v49	1013.7283	23.5805	1020.1862	34.8568	1019.4537	124.7664
v50	1027.9360	164.1262	1033.2915	58.5700	1032.0588	100.2375
v51	1053.4163	30.3871	1047.6848	10.2488	1052.7959	13.7909
v52	1068.2801	127.6981	1061.8736	35.4667	1063.5256	149.3232
v53	1090.4657	37.6113	1070.0522	126.5585	1071.7386	126.2499
v54	1098.5320	352.4970	1095.7925	100.6217	1095.9000	124.9046
v55	1111.1321	15.9902	1102.3730	7.6935	1101.7395	17.6266
v56	1113.6871	74.6341	1108.6666	172.2745	1111.7089	16.3283
v57	1115.0000	34.9827	1116.6044	100.7428	1119.3173	180.9165
v58	1128.8657	76.4865	1139.2581	40.2475	1135.7705	86.5460
v59	1149.2034	30.3062	1151.9980	20.2452	1147.6528	69.7988
v60	1158.9314	27.2260	1154.1105	41.7890	1148.8056	3.8090
v61	1188.6297	3.1875	1189.8114	0.0635	1189.0233	3.3216
v62	1202.4627	0.6740	1193.5681	13.1306	1207.2021	20.8943
v63	1207.6978	15.2745	1212.3958	2.1510	1218.0740	39.0068
v64	1229.6858	40.2026	1217.1487	11.2755	1223.0919	17.8781
v65	1235.4750	36.0897	1237.0374	28.2797	1237.5579	58.5921
v66	1251.2511	281.2179	1238.1931	174.7998	1249.7158	236.7888
v67	1282.2996	51.1930	1263.4361	26.8331	1261.7409	22.3039
v68	1300.2607	35.1934	1298.2760	16.0480	1286.3017	65.0234
v69	1316.6194	5.0760	1328.9803	59.0662	1305.9967	1.8581
v70	1331.3298	18.2599	1333.8879	5.0019	1334.8957	17.4904
v71	1346.2782	2.3664	1347.4340	11.3071	1347.0145	3.3422
v72	1360.9922	49.2238	1352.1938	1.6186	1352.1405	3.8408
v73	1367.5228	4.7986	1359.0677	0.7449	1367.2546	5.4650
v74	1374.0871	21.9388	1359.6767	26.6867	1377.2987	50.9158
v75	1391.0481	6.6618	1374.3687	18.6267	1391.1472	18.8089

v76	1398.1319	18.2561	1392.8334	5.9468	1396.7648	21.6679
v77	1409.7190	7.6636	1403.1226	14.6077	1399.5567	17.2811
v78	1414.4487	3.3503	1418.5374	6.0136	1411.9804	5.3558
v79	1438.1129	11.1891	1434.2163	24.2649	1435.7335	23.3363
v80	1443.7776	24.3579	1438.6730	4.1496	1442.2346	35.9531
v81	1462.4523	58.2279	1456.4331	11.7389	1458.7728	18.9573
v82	1491.7444	52.2195	1482.2847	47.7335	1469.5737	25.8376
v83	1498.8744	0.8642	1493.2116	1.4994	1498.7544	0.6690
v84	1531.4649	1.4536	1517.2498	2.0114	1517.0425	2.4268
v85	1536.7454	97.9210	1533.6872	70.4504	1536.8800	96.8289
v86	1640.8927	24.6497	1641.1418	7.5852	1641.2342	26.0126
v87	1652.3142	60.4227	1645.8743	38.3058	1652.6025	61.2409
v88	2599.5444	137.3262	2645.2061	78.2921	2582.3817	171.8586
v89	2793.9934	99.4548	2801.7149	95.5278	2791.9286	101.7912
v90	2998.0467	40.7701	3001.1642	10.3456	2992.7618	12.7061
v91	3011.3433	23.9360	3016.1528	46.4510	3013.2169	45.9531
v92	3040.9884	17.8867	3025.7608	24.1366	3019.4495	35.7763
v93	3064.3354	30.4368	3066.7181	25.5756	3073.3934	24.6227
v94	3091.5002	13.3554	3079.2075	34.2696	3091.0914	17.1562
v95	3101.1052	27.1382	3108.6557	21.0077	3108.7432	21.0220
v96	3111.5106	30.7986	3146.7994	9.4567	3146.7408	8.3090
v97	3185.6507	1.5413	3185.8019	1.2879	3186.5806	1.7906
v98	3193.2209	9.8627	3194.2251	5.9846	3193.9521	9.2044
v99	3204.6756	23.6120	3202.5579	17.7988	3205.6484	21.3619
v100	3212.9842	14.9722	3210.9975	17.0924	3213.8205	15.1088
v101	3235.0817	0.8641	3220.3017	2.1584	3232.0706	3.6395
v102	3467.5025	836.0122	3518.9744	422.3207	3510.6362	642.2794
v103	3661.0581	117.3300	3723.3556	45.3183	3688.2095	84.0624
v104	3703.6515	63.0972	3730.7385	57.7630	3709.9849	57.1276
v105	3707.4583	49.3549	3734.9981	25.1088	3746.1561	25.5062

Table 3. α -PhGlc $\cdot$ (D₂O)₂

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	6.70	0.00
B	5.42	6.62
C	0.00	6.69
D	5.62	7.57



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.309142	-1.513750	-0.777202
6	1.698280	-1.994469	-0.340893
6	2.419782	-0.897652	0.441424
6	2.468698	0.407274	-0.366475
6	1.041115	0.772340	-0.798409
8	0.440449	-0.321418	-1.531394
8	1.570350	-3.196842	0.396032
8	3.729265	-1.388784	0.723650
8	3.091934	1.442877	0.380106
6	0.938399	1.989680	-1.700552
8	-0.431620	2.394801	-1.862016
1	2.447938	-3.402196	0.760088
1	4.230885	-0.659886	1.127101
1	-0.914915	1.642513	-2.243996
1	-0.160722	-2.242781	-1.444636
1	2.261063	-2.178020	-1.269754
1	1.881645	-0.713564	1.382635
1	3.098537	0.250268	-1.251307
1	0.441078	0.955551	0.099836
1	2.457522	1.793787	1.048899
1	1.456791	2.836988	-1.248591
1	1.387577	1.780490	-2.680210
8	-0.480913	-1.318892	0.379599
6	-3.880142	-0.642729	-0.947216
6	-2.514990	-0.955088	-0.957095
6	-1.815260	-1.011942	0.255149
6	-2.478399	-0.741936	1.461454
6	-3.836386	-0.424874	1.453593
6	-4.547565	-0.372741	0.248232
1	-4.418341	-0.606710	-1.891188
1	-2.015178	-1.143239	-1.900251
1	-1.915462	-0.799527	2.388529
1	-4.342203	-0.224959	2.394895
1	-5.605594	-0.126917	0.243959
8	-1.271085	2.902039	0.808280
1	-1.108947	2.815136	-0.159029
1	-1.937484	2.229561	1.024070
8	1.139697	2.502575	2.130447
1	0.260389	2.703047	1.723761
1	1.374769	3.274921	2.665501

B			
6	0.145632	0.065148	1.107863
6	-1.267490	-0.493298	1.301113
6	-2.182314	-0.053074	0.153915
6	-2.178615	1.474952	0.072044
6	-0.739515	1.968028	-0.110012
8	0.089103	1.466572	0.967081
8	-1.191236	-1.916149	1.426549
8	-3.514606	-0.506957	0.365119
8	-2.952510	1.929686	-1.029035
6	-0.594465	3.483590	-0.068373
8	0.754143	3.887031	-0.275993
1	-2.088626	-2.234963	1.626253
1	-3.658488	-1.302421	-0.195163
1	1.293594	3.450555	0.403871
1	0.769303	-0.113491	1.989144
1	-1.653040	-0.073285	2.239963
1	-1.801838	-0.452959	-0.794310
1	-2.586038	1.881350	1.012634
1	-0.348935	1.597962	-1.066322
1	-3.802825	1.459041	-0.980781
1	-1.183505	3.925456	-0.874802
1	-0.974048	3.863261	0.892861
8	0.725469	-0.575730	-0.024121
6	4.148113	0.363364	-1.012529
6	2.754784	0.389237	-0.900982
6	2.117229	-0.557447	-0.096993
6	2.851381	-1.525987	0.592580
6	4.244104	-1.540313	0.477826
6	4.894898	-0.597127	-0.323630
1	4.648317	1.098357	-1.637721
1	2.163933	1.132477	-1.427296
1	2.330088	-2.262227	1.198416
1	4.818553	-2.294262	1.009802
1	5.977738	-0.612904	-0.413237
8	-0.727201	-3.313555	-0.971937
1	-0.095122	-2.863958	-1.553248
1	-0.671532	-2.824429	-0.119884
8	-3.417824	-2.826825	-1.134229
1	-2.475770	-3.106859	-1.250136
1	-3.946912	-3.281728	-1.804446

C			
6	0.810471	0.473363	-0.959460
6	-0.112708	1.688721	-1.102685
6	-0.989530	1.827895	0.137885
6	-1.781801	0.541036	0.379122
6	-0.807543	-0.650695	0.451394
8	0.026191	-0.691994	-0.731263
8	0.667313	2.843408	-1.353699
8	-1.852164	2.941105	-0.088409
8	-2.494485	0.680681	1.599349
6	-1.476263	-2.017727	0.506135
8	-2.160655	-2.331822	-0.716915
1	0.071564	3.607977	-1.278313
1	-2.456414	2.993446	0.671509
1	-1.559941	-2.104348	-1.448106
1	1.354517	0.282399	-1.889550
1	-0.766499	1.482192	-1.965118
1	-0.355048	2.023348	1.013768
1	-2.477710	0.397067	-0.459065
1	-0.179014	-0.537641	1.344574
1	-3.435913	0.421924	1.464805
1	-0.721733	-2.789070	0.705795
1	-2.223501	-2.037734	1.302670
8	1.713135	0.715250	0.092745
6	4.371024	-1.826906	-0.375403
6	3.123612	-1.204092	-0.503055
6	2.901118	0.015290	0.146653
6	3.906126	0.594423	0.930856
6	5.138540	-0.043830	1.057423
6	5.380534	-1.256868	0.401433
1	4.542899	-2.772767	-0.883299
1	2.336292	-1.674962	-1.080964
1	3.705304	1.543180	1.419311
1	5.916129	0.412942	1.664416
1	6.343595	-1.750511	0.497930
8	-4.880536	-1.913312	-0.888982
1	-5.355469	-2.740687	-1.052144
1	-3.918216	-2.128623	-0.893762
8	-5.115742	-0.041538	1.109093
1	-5.181017	-0.736288	0.410190
1	-5.645769	-0.349737	1.858226

D			
6	-0.547009	-0.367751	-0.802459
6	0.571647	-1.414850	-0.763240
6	1.246117	-1.409175	0.611752
6	1.742852	-0.002039	0.944090
6	0.641831	1.050636	0.762043
8	0.007399	0.914311	-0.527308
8	0.051543	-2.688127	-1.097079
8	2.309710	-2.358954	0.670953
8	2.198527	0.091489	2.291883
6	1.183910	2.476835	0.789409
8	2.036765	2.745405	-0.335902
1	0.697504	-3.344684	-0.782733
1	3.037857	-2.054756	0.081523
1	1.517499	2.545759	-1.134202
1	-0.979708	-0.288456	-1.804574
1	1.309008	-1.100297	-1.519395
1	0.522283	-1.732656	1.366854
1	2.565646	0.236814	0.259394
1	-0.103525	0.934901	1.559644
1	2.740596	-0.697124	2.465904
1	0.351870	3.191990	0.792893
1	1.789232	2.627097	1.685456
8	-1.535804	-0.728572	0.131440
6	-4.477688	1.320146	-0.814973
6	-3.141789	0.906253	-0.750062
6	-2.816388	-0.231744	-0.003580
6	-3.811148	-0.935485	0.686009
6	-5.134719	-0.504151	0.620683
6	-5.477440	0.624172	-0.134079
1	-4.728635	2.203184	-1.397534
1	-2.370412	1.477024	-1.254740
1	-3.528961	-1.816772	1.254164
1	-5.902982	-1.057143	1.155185
1	-6.510614	0.956097	-0.186983
8	4.528575	1.566003	-0.890140
1	3.697825	2.031506	-0.634885
1	5.241656	1.985820	-0.386794
8	4.346786	-1.214636	-0.952366
1	4.748715	-1.554727	-1.764586
1	4.476083	-0.236017	-0.959999

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	18.1796	0.2292	12.2429	24.9602	21.7309	0.5471
v2	34.5675	0.0633	17.7849	14.0301	27.5085	1.8034
v3	42.9419	0.6374	29.7438	2.3619	33.7893	0.8690
v4	44.0835	0.2520	32.1483	5.8572	36.6850	0.0262
v5	49.6417	1.1484	39.8541	10.8906	46.7540	0.1349
v6	81.0059	4.5710	51.7897	4.0734	70.3980	5.3365
v7	100.4478	0.4202	68.9729	9.7488	99.8537	2.5798
v8	110.2601	9.4478	94.9499	2.1871	101.9404	3.0873
v9	121.4688	2.2092	108.7664	2.4771	111.7250	1.7082
v10	138.7359	0.7305	120.1926	1.2076	143.8928	2.4292
v11	169.9974	29.3974	123.9121	3.3721	154.8234	59.7007
v12	177.0267	13.2387	153.0811	3.6492	169.2056	23.6315
v13	187.8939	1.8525	190.0142	9.6398	189.5150	46.7450
v14	203.7816	9.7865	202.4901	17.6964	192.2784	2.0844
v15	210.4833	1.3292	214.6995	6.7791	206.9570	11.3441
v16	240.8995	17.7424	231.3148	19.5545	229.0358	6.4695
v17	245.5944	10.0646	237.5137	23.6518	250.1493	22.2067
v18	248.4812	37.0709	253.6272	7.1839	255.7199	10.2481
v19	253.8001	51.2199	257.5789	14.5057	261.6647	31.1252
v20	261.7431	24.7874	263.9548	43.0065	269.4897	10.9356
v21	304.3715	7.2880	275.1442	33.6138	290.3514	9.6349
v22	313.0259	9.4542	318.3074	5.0149	310.8236	41.3026
v23	343.0196	2.9954	353.0546	4.0634	334.0622	14.9000
v24	361.7406	77.2222	371.8890	61.0424	355.1021	2.1073
v25	368.3045	15.6890	386.8126	0.3603	373.3146	133.4355
v26	381.3008	54.0464	401.1023	32.4965	384.4372	20.9422
v27	406.9291	58.0765	417.6187	31.1048	399.2515	53.9431
v28	410.7305	17.1436	423.6674	64.1243	416.6137	49.5962
v29	420.4242	2.3846	430.6799	189.8740	424.0836	0.5369
v30	427.0851	22.1905	439.4019	18.2559	436.6123	58.6228
v31	447.5099	4.3915	453.0601	15.6970	456.0402	87.0016
v32	495.8985	90.2160	468.6625	148.8847	502.7572	1.0834
v33	517.1636	27.5988	499.7855	7.5146	516.8642	8.3314
v34	518.3385	138.4041	536.0162	8.6802	523.6647	23.7590
v35	533.6054	2.3963	558.6448	3.8059	532.0558	18.9719
v36	552.4407	11.8085	567.9785	82.2386	546.6356	28.3790
v37	585.5843	13.9491	580.6230	11.9189	571.5501	19.8612
v38	611.9318	18.2594	590.6155	44.5585	619.2685	5.6054
v39	627.6077	3.1191	607.6850	21.4157	625.5974	39.5399
v40	630.6484	58.4282	628.9335	0.1270	638.5433	31.9069
v41	684.7725	31.7027	663.5977	16.1231	699.8041	15.0985
v42	696.5927	15.6548	707.2676	34.9295	708.2253	27.5448
v43	740.5549	90.5795	738.4161	7.5002	750.2439	2.6533
v44	746.6258	52.9114	777.0162	26.8894	757.0601	106.9815
v45	764.0988	72.9936	780.7394	29.7877	765.5761	64.4631
v46	832.5218	2.0256	836.2612	22.5978	838.7192	0.4877
v47	840.5964	1.6747	848.2301	1.4242	856.4959	23.6724
v48	861.6462	59.3195	867.4098	59.3085	876.8239	32.6646
v49	902.0526	5.6485	913.0896	28.6442	907.4347	6.3885
v50	937.3010	32.4731	942.2280	16.1668	923.0011	9.5110
v51	972.9138	0.5181	978.6141	0.5609	940.5595	31.0459
v52	992.4111	0.0892	999.3659	11.7439	971.0000	0.3415
v53	1000.7047	50.0411	1006.7941	29.5392	991.6229	0.0912
v54	1012.1831	4.4996	1009.5366	182.4133	1013.5890	28.5984
v55	1027.8545	214.7163	1021.9473	67.0838	1018.9603	60.8228
v56	1037.8886	83.3602	1032.5676	48.2293	1032.9735	397.2679
v57	1045.1973	46.3922	1047.9914	13.2220	1039.7124	109.7761
v58	1053.1260	20.3757	1060.7676	159.4345	1052.6189	44.8288
v59	1060.1799	192.2357	1067.6931	105.0510	1065.9700	174.8704
v60	1095.5762	13.2215	1093.4961	90.2434	1100.9820	6.3816
v61	1109.1594	14.7052	1101.9158	8.9499	1108.2626	6.9455
v62	1116.9834	54.9735	1108.5744	47.4205	1115.1823	44.2207
v63	1122.8273	75.0875	1124.5727	125.1974	1118.9291	59.6311
v64	1131.8129	136.9486	1138.2275	77.8848	1124.4196	68.9094
v65	1145.3030	14.8580	1139.9157	22.4595	1143.1160	80.8129
v66	1157.5631	7.0362	1152.2554	5.8112	1148.8004	21.5702
v67	1187.8003	3.0775	1189.1868	0.1902	1187.3601	2.9096
v68	1207.6171	21.3628	1195.1230	13.7066	1203.4970	18.2590
v69	1219.7860	7.4148	1220.1845	11.7753	1223.7776	52.6210
v70	1231.0395	68.8122	1229.9704	26.4637	1236.7017	21.4119
v71	1246.0668	61.3043	1235.6029	202.5015	1242.1644	41.6865
v72	1262.1448	69.8623	1246.2841	80.3907	1255.0605	37.4448
v73	1264.7411	190.9809	1250.2699	11.3334	1261.6864	273.6422
v74	1267.4255	21.1603	1271.6446	23.3499	1267.0578	5.2419
v75	1276.3235	19.6021	1279.7465	31.9406	1269.9853	38.9333

v76	1305.3332	24.8518	1317.0748	12.4517	1314.1309	35.1486
v77	1343.4814	7.2198	1333.4308	1.0831	1341.8802	3.0862
v78	1353.6725	19.5661	1348.7951	11.2717	1344.6813	11.4045
v79	1363.3135	17.1336	1353.5700	0.9778	1362.2998	10.7369
v80	1368.0260	6.6716	1359.1271	0.5491	1365.4050	17.3510
v81	1376.4498	3.4059	1372.6927	28.0362	1368.6485	6.1320
v82	1393.5999	3.5448	1393.5099	12.2821	1380.8584	12.6376
v83	1401.8094	10.8063	1400.2951	3.1247	1401.3275	23.9059
v84	1403.6129	47.6474	1409.0459	47.2356	1410.7091	45.6228
v85	1418.3995	5.1541	1418.6752	11.2283	1425.3064	13.3391
v86	1443.4662	32.3852	1434.5765	31.1124	1437.1313	43.6048
v87	1449.6216	14.0455	1437.6660	14.2999	1443.4309	14.1349
v88	1450.7968	2.6791	1456.0789	6.1739	1453.0981	20.4575
v89	1492.0979	59.8189	1472.6575	16.8536	1490.4099	19.0135
v90	1496.8564	0.5361	1492.4837	1.6958	1497.7184	0.5867
v91	1515.9173	3.8155	1517.2567	1.9629	1522.2482	7.6446
v92	1536.4421	99.0814	1534.3159	71.8855	1536.5375	104.3135
v93	1635.8106	23.5886	1640.3563	6.0396	1638.0238	21.8743
v94	1650.7842	71.0813	1645.9849	41.0014	1652.6847	71.4588
v95	2478.6927	299.5955	2473.4427	298.6983	2495.1821	289.1689
v96	2549.0316	173.8360	2565.3783	227.0052	2537.5119	386.4357
v97	2760.1328	66.5604	2779.7576	49.1331	2787.8694	62.2249
v98	2784.1672	64.2266	2796.0417	73.8464	2792.5523	95.3340
v99	3008.7606	20.2768	2994.5489	18.5374	3003.1393	25.8131
v100	3035.8526	16.0850	3015.4627	49.2945	3035.6392	1.3765
v101	3054.4219	21.4809	3045.2161	14.2161	3047.5590	28.2458
v102	3062.8767	31.4261	3062.7443	3.5320	3054.8435	11.4680
v103	3088.7691	34.7993	3070.4239	55.2454	3066.3135	61.7930
v104	3098.6818	28.3478	3098.8700	22.3289	3100.0916	22.0359
v105	3156.1917	7.5534	3144.6599	10.0976	3142.3223	12.8618
v106	3184.9103	1.8896	3185.1430	0.7344	3182.3147	1.4459
v107	3192.1451	12.9482	3193.9876	8.5973	3190.9195	15.9285
v108	3208.1210	20.7205	3203.6420	21.3071	3205.9005	29.9929
v109	3214.8675	7.4296	3211.0635	14.9159	3215.7448	6.8434
v110	3230.7203	4.6159	3220.2644	2.3968	3228.2428	3.0716
v111	3466.9905	453.3436	3509.5559	662.2241	3457.8816	983.0648
v112	3723.7384	49.3065	3711.1846	40.8560	3718.0051	56.5270
v113	3728.3849	57.4371	3719.7107	63.4729	3726.3231	49.1804
v114	3729.3807	38.7655	3736.1914	27.1173	3727.6717	57.4641

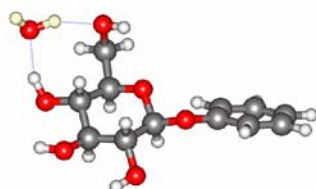
D		
	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	25.2654	0.5333
v2	33.3189	1.2695
v3	36.5537	2.4949
v4	44.7792	0.1594
v5	50.6744	0.2213
v6	72.6626	9.1855
v7	94.1309	33.7610
v8	102.0424	2.4071
v9	109.6256	5.8647
v10	119.2193	25.3352
v11	142.2330	0.4272
v12	158.3187	60.6086
v13	185.8782	17.2636
v14	191.3411	9.5669
v15	204.6877	14.5467
v16	209.1665	15.5042
v17	244.4066	13.6794
v18	253.8203	4.2695
v19	259.5898	22.5125
v20	265.6945	3.7564
v21	282.9607	19.3989
v22	313.6535	37.3395
v23	333.0602	7.5276
v24	341.5538	15.9430
v25	355.1738	7.2429
v26	365.2899	33.3712
v27	405.4088	136.0603
v28	415.4265	16.7053
v29	423.4199	0.0954
v30	444.2513	12.8112
v31	485.9169	140.7701
v32	506.1900	15.9238
v33	517.7311	15.8389
v34	524.2936	14.7697
v35	533.4632	9.8821
v36	551.8396	19.4694
v37	573.4030	25.0971
v38	591.1037	91.8180
v39	623.0864	6.2267
v40	640.4491	17.0439
v41	700.0487	19.6513
v42	711.0037	11.4274
v43	752.4211	4.7847
v44	765.6673	63.9286
v45	803.8348	134.9628
v46	838.2301	0.2679
v47	855.8161	34.3340
v48	883.1669	38.4902
v49	906.9955	4.8479
v50	917.5370	9.4014
v51	952.0941	13.2386
v52	971.2043	0.4256
v53	991.9620	0.1139
v54	1014.1877	6.9302
v55	1016.6779	78.8287
v56	1031.3532	257.1460
v57	1036.8239	169.1545
v58	1052.7039	69.2779
v59	1067.2479	198.8835
v60	1094.6042	58.2611
v61	1099.7940	44.8472
v62	1108.4383	8.3155
v63	1118.6988	43.3616
v64	1134.5136	70.0115
v65	1140.9818	39.7352
v66	1151.7702	26.6984
v67	1187.5007	2.9859
v68	1204.6015	14.9422
v69	1227.3363	34.2811
v70	1246.0616	45.2833
v71	1249.1954	66.1448
v72	1257.1201	12.2196
v73	1262.2851	201.9394
v74	1263.6239	108.0338
v75	1290.0789	39.5654

v76	1313.4040	39.4511
v77	1340.6194	11.7808
v78	1343.0688	4.7998
v79	1353.7935	10.9856
v80	1366.3414	2.1883
v81	1370.3703	6.0933
v82	1385.8178	4.2452
v83	1399.7136	42.1769
v84	1415.8653	23.6885
v85	1427.5545	1.8380
v86	1432.8912	24.8003
v87	1437.9556	46.8293
v88	1459.4341	8.0311
v89	1483.8933	40.9881
v90	1497.7877	0.5127
v91	1517.4983	7.7048
v92	1536.4597	103.7328
v93	1638.1660	21.8842
v94	1652.7023	71.5934
v95	2501.6125	350.5315
v96	2541.4560	256.5613
v97	2784.5734	86.8648
v98	2790.6273	62.4831
v99	3001.0883	31.2157
v100	3054.2057	9.8838
v101	3064.4768	21.8264
v102	3073.0690	30.7754
v103	3097.7155	16.9848
v104	3101.1906	36.4505
v105	3152.6007	7.7540
v106	3182.4444	1.5756
v107	3190.7927	15.5782
v108	3206.0779	29.4266
v109	3215.2777	7.2458
v110	3227.3358	3.1819
v111	3501.8245	454.6399
v112	3704.4244	43.4370
v113	3717.6877	57.0840
v114	3721.3466	41.0642

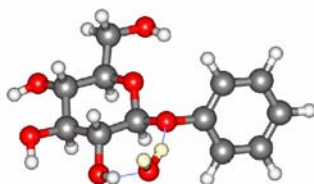
Table 4. β -PhGlc $\cdot$ D₂O

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

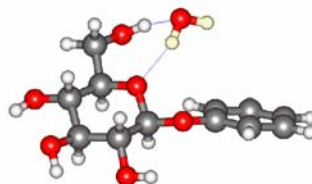
Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	0.00	0.00
B	5.95	0.99
C	4.88	1.11
D	7.62	2.28
E	0.15	3.58
F	6.56	4.00



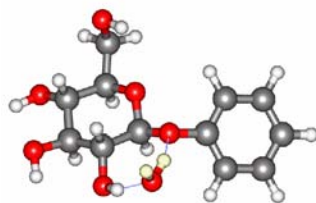
A



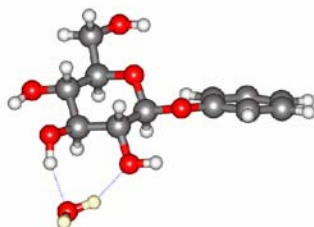
B



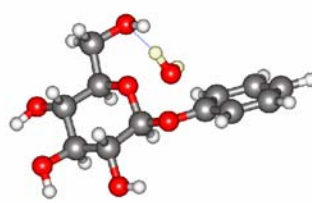
C



D



E



F

(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	-0.465449	0.637753	-0.130219
6	0.463329	1.792641	0.257369
6	1.808880	1.646214	-0.452141
6	2.416903	0.269156	-0.207116
6	1.403686	-0.793445	-0.673287
8	0.184938	-0.621708	0.067649
8	-0.174461	3.008265	-0.103109
8	2.648327	2.691799	0.028783
8	3.646987	0.204256	-0.913384
6	1.835924	-2.236561	-0.448459
8	2.143900	-2.515354	0.924381
1	0.477314	3.719169	0.017381
1	3.529097	2.545780	-0.357264
1	1.377698	-2.251892	1.462171
1	0.622646	1.746967	1.345082
1	1.654760	1.772595	-1.536731
1	2.590087	0.144893	0.869992
1	1.215040	-0.662984	-1.752540
1	4.246962	-0.392979	-0.416298
1	1.042117	-2.910453	-0.794985
1	2.746367	-2.446742	-1.014504
8	-1.579143	0.678163	0.705514
1	-0.770637	0.730691	-1.184687
6	-5.250858	-1.010256	-0.346013
6	-5.147670	-0.029322	0.647454
6	-3.908744	0.520365	0.972584
6	-2.759018	0.082961	0.305096
6	-2.844693	-0.906733	-0.679478
6	-4.097312	-1.440938	-1.003107
1	-6.218162	-1.434544	-0.600429
1	-6.037601	0.316529	1.167200
1	-3.811285	1.292166	1.730092
1	-1.951217	-1.278001	-1.168211
1	-4.161574	-2.209397	-1.769571
8	4.797801	-1.711942	0.778147
1	3.961370	-2.097258	1.118960
1	5.410361	-1.643383	1.524375

B			
6	-0.145646	0.413205	0.147766
6	-1.297618	1.397462	-0.103782
6	-2.588554	0.794772	0.456057
6	-2.843956	-0.609556	-0.084119
6	-1.611462	-1.482971	0.176784
8	-0.459378	-0.850716	-0.412977
8	-1.123344	2.643969	0.546061
8	-3.719604	1.594931	0.126210
8	-3.962221	-1.212544	0.555061
6	-1.697428	-2.870672	-0.445771
8	-0.542725	-3.647740	-0.157675
1	-0.497143	3.192712	0.025121
1	-3.527045	2.500154	0.425068
1	0.232109	-3.128537	-0.429462
1	-1.400178	1.527259	-1.191498
1	-2.491770	0.732585	1.552300
1	-3.015475	-0.545829	-1.170455
1	-1.455640	-1.586219	1.261978
1	-4.693291	-0.572568	0.523577
1	-2.552095	-3.405086	-0.025884
1	-1.844510	-2.771552	-1.532677
8	1.021008	0.885047	-0.498812
1	0.049112	0.308242	1.226896
6	4.666836	-0.881411	0.536349
6	4.000800	-1.275211	-0.628529
6	2.772197	-0.700991	-0.966596
6	2.223215	0.269643	-0.128927
6	2.879216	0.680053	1.032237
6	4.105173	0.095761	1.363675
1	5.621109	-1.331360	0.796223
1	4.435779	-2.032337	-1.275687
1	2.237092	-0.991199	-1.865405
1	2.437597	1.452886	1.655352
1	4.623129	0.411408	2.265403
8	0.913329	3.656117	-1.067256
1	0.845981	3.982437	-1.976678
1	1.202096	2.724002	-1.119936

C			
6	-0.167020	-0.747074	-0.085394
6	-1.275433	-1.717392	0.329973
6	-2.593705	-1.261277	-0.290040
6	-2.888247	0.202771	0.040854
6	-1.690561	1.085744	-0.341067
8	-0.514150	0.568499	0.324375
8	-1.033814	-3.040317	-0.138086
8	-3.697992	-2.028047	0.182653
8	-4.025759	0.662900	-0.676311
6	-1.865777	2.548587	0.066636
8	-0.806476	3.370764	-0.385331
1	-0.237680	-3.381963	0.299976
1	-3.527062	-2.961760	-0.024063
1	-0.073613	3.303604	0.260936
1	-1.353654	-1.699688	1.426076
1	-2.517055	-1.361469	-1.384603
1	-3.061376	0.288250	1.125344
1	-1.529741	1.042412	-1.428933
1	-4.743410	0.025389	-0.523091
1	-2.788118	2.913062	-0.393934
1	-1.981919	2.610169	1.159422
8	1.005154	-1.133709	0.577724
1	-0.013540	-0.772807	-1.175927
6	4.806468	0.038100	-0.705897
6	3.689611	0.712620	-1.201102
6	2.396421	0.358207	-0.796208
6	2.234304	-0.696909	0.107770
6	3.346454	-1.378750	0.613638
6	4.627303	-1.007469	0.207351
1	5.805119	0.323673	-1.023859
1	3.813523	1.531116	-1.905483
1	1.543094	0.915464	-1.166558
1	3.191088	-2.190230	1.318605
1	5.487735	-1.540932	0.602701
8	1.023225	2.584609	1.648826
1	0.689789	1.698220	1.409013
1	1.976395	2.556933	1.474501

D			
6	0.034617	0.319948	-0.168227
6	1.082905	1.406998	0.107745
6	2.379867	1.019851	-0.604334
6	2.843546	-0.378535	-0.210625
6	1.709370	-1.386960	-0.436808
8	0.523143	-0.945705	0.250251
8	0.708600	2.679541	-0.390071
8	3.432235	1.927818	-0.294370
8	3.947788	-0.794207	-1.007883
6	2.011151	-2.783222	0.102335
8	2.179709	-2.796347	1.514197
1	0.085274	3.096266	0.243453
1	3.102759	2.822690	-0.485412
1	1.380371	-2.407134	1.905270
1	1.260367	1.443121	1.192935
1	2.193160	1.033868	-1.690912
1	3.118713	-0.382715	0.853303
1	1.508053	-1.461607	-1.517872
1	4.628102	-0.103414	-0.943451
1	1.199770	-3.461809	-0.200173
1	2.948774	-3.140938	-0.329213
8	-1.134205	0.594398	0.579155
1	-0.219463	0.288812	-1.239524
6	-4.730590	-1.124582	-0.686051
6	-4.390842	0.172061	-1.083174
6	-3.179336	0.738053	-0.675884
6	-2.317361	-0.006382	0.130437
6	-2.644097	-1.299837	0.539525
6	-3.856685	-1.856837	0.123774
1	-5.673666	-1.561549	-1.003061
1	-5.068473	0.747393	-1.708392
1	-2.900906	1.746449	-0.968819
1	-1.953755	-1.850351	1.169213
1	-4.118820	-2.864060	0.437006
8	-1.236578	3.253989	1.534754
1	-1.105379	3.483700	2.466492
1	-1.405689	2.292041	1.498623

E			
6	-0.062790	-0.269925	-0.061219
6	1.182782	-1.062595	-0.476303
6	2.430296	-0.399847	0.116515
6	2.452594	1.092253	-0.242226
6	1.137944	1.772828	0.149945
8	0.046826	1.075112	-0.482524
8	1.084003	-2.409607	0.006951
8	3.646457	-0.941246	-0.372842
8	3.517690	1.748240	0.428548
6	1.041723	3.222800	-0.310198
8	-0.200726	3.810394	0.053816
1	0.250473	-2.780772	-0.328100
1	3.816478	-1.803469	0.068576
1	-0.903267	3.296077	-0.376435
1	1.248588	-1.061590	-1.572235
1	2.388978	-0.493872	1.213655
1	2.581585	1.177401	-1.333314
1	1.009237	1.734072	1.243176
1	4.309581	1.198689	0.293236
1	1.823581	3.808635	0.177236
1	1.195389	3.270389	-1.399094
8	-1.156107	-0.869354	-0.703598
1	-0.197626	-0.314224	1.032680
6	-5.104903	-0.295822	0.537802
6	-4.108067	0.532469	1.055380
6	-2.772726	0.383247	0.662700
6	-2.442462	-0.621809	-0.251169
6	-3.433420	-1.455056	-0.781327
6	-4.760039	-1.288130	-0.386812
1	-6.138840	-0.167684	0.845355
1	-4.363023	1.314340	1.766097
1	-2.016749	1.057162	1.048725
1	-3.150271	-2.221104	-1.497510
1	-5.525881	-1.938141	-0.802005
8	3.536877	-3.430763	0.879258
1	2.592305	-3.392188	0.622653
1	3.913687	-4.208410	0.441914

F			
6	0.123997	-0.762060	0.075736
6	1.238711	-1.809843	-0.020947
6	2.560547	-1.192254	0.430977
6	2.852742	0.097906	-0.335438
6	1.651712	1.043426	-0.214847
8	0.476687	0.373652	-0.703093
8	0.996379	-2.930754	0.823391
8	3.662917	-2.069623	0.213047
8	3.996967	0.761626	0.186188
6	1.790367	2.311096	-1.049690
8	0.611456	3.119902	-0.961949
1	0.177849	-3.362625	0.529231
1	3.481139	-2.900886	0.681970
1	-0.123372	2.591605	-1.319237
1	1.317407	-2.125306	-1.071062
1	2.487053	-0.952364	1.503574
1	3.008817	-0.152639	-1.396596
1	1.502229	1.319418	0.839320
1	4.711986	0.105649	0.244410
1	2.616861	2.916460	-0.673691
1	1.989509	2.051776	-2.098534
8	-1.029138	-1.338984	-0.462361
1	-0.041836	-0.463054	1.122368
6	-4.870972	0.181651	0.167341
6	-4.654294	-1.014994	-0.525314
6	-3.358770	-1.491701	-0.719454
6	-2.270619	-0.767488	-0.220015
6	-2.466604	0.435321	0.464726
6	-3.775457	0.895206	0.655743
1	-5.880750	0.552895	0.319219
1	-5.495741	-1.581888	-0.915629
1	-3.173114	-2.418558	-1.254686
1	-1.641574	1.028682	0.843585
1	-3.924087	1.829755	1.190411
8	-0.396718	2.959507	1.675280
1	-0.030015	3.247671	0.812162
1	-0.458904	3.753197	2.226245

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	25.8758	0.1587	22.7192	0.2079	29.8910	0.3335
v2	40.1831	1.0483	32.3656	0.2390	41.2449	1.6739
v3	43.6884	1.5493	40.3039	1.1479	50.7485	0.5908
v4	60.6569	0.8484	50.9696	0.3046	57.6656	0.4435
v5	83.9200	5.0654	79.8774	0.8703	85.9511	0.6816
v6	94.7907	5.4611	102.7150	5.3292	97.4355	8.5345
v7	116.6414	1.5634	105.8563	1.8903	113.3305	1.3560
v8	126.7999	60.5732	133.5033	12.1539	136.4775	5.9479
v9	148.4439	1.2614	143.7360	3.2832	162.3180	2.6324
v10	182.3143	37.0892	157.4623	3.7246	187.2140	25.6183
v11	205.9652	1.9874	181.8571	15.9523	198.7311	1.4510
v12	217.1173	21.9396	186.7383	59.0029	208.3773	5.8684
v13	228.1785	1.3738	213.9564	3.8327	217.5600	25.4393
v14	243.8221	7.1579	222.8925	41.2317	240.0346	6.9916
v15	261.0868	6.9383	232.7617	6.5511	246.4122	6.2027
v16	265.0583	11.0471	243.4993	5.4761	266.8141	12.5826
v17	288.6954	2.8219	286.2783	19.5879	281.3574	24.7139
v18	300.1546	14.4903	311.7888	5.4961	287.7712	24.2612
v19	323.3868	8.1179	345.7487	12.4877	310.7961	2.5077
v20	345.4050	21.8632	372.8319	0.8152	345.4614	19.1304
v21	384.1011	107.1933	396.9963	31.4026	367.4091	120.0134
v22	408.7700	63.6242	415.1297	175.4915	390.2544	15.6650
v23	421.3923	0.3938	418.4854	29.4616	396.4123	131.8908
v24	424.9438	35.5263	425.2976	3.2010	403.3215	42.8922
v25	434.3587	34.9557	428.2090	19.4973	405.8267	130.0959
v26	444.2810	60.1538	430.3723	160.5110	424.7198	0.2135
v27	466.3099	34.1842	440.5391	2.7308	429.3696	0.5115
v28	481.4379	127.4549	445.3973	41.1541	474.8329	1.9429
v29	515.2685	6.9208	493.8318	4.6206	502.8755	7.5623
v30	534.3475	11.0550	531.6068	14.3044	520.3970	6.4576
v31	545.8670	19.3621	539.3186	7.2108	540.2160	8.6048
v32	577.9379	2.6350	594.4986	19.8884	594.5037	30.3272
v33	621.4768	6.8670	625.2618	0.9029	620.3667	3.2016
v34	634.9307	10.7982	634.2345	16.5249	634.2230	22.6388
v35	648.7571	27.2316	639.5699	1.7695	644.6740	4.5581
v36	696.8081	21.5224	644.7997	15.5735	650.1204	18.9970
v37	715.1863	1.2035	707.3882	39.1702	692.8295	32.5195
v38	742.6389	102.7588	770.4279	116.0162	710.0261	150.1288
v39	764.4799	64.8022	785.1745	54.3098	764.8240	66.8320
v40	834.0353	9.9170	840.9661	14.8213	834.2689	27.4283
v41	838.2250	17.5939	847.9507	0.1349	843.0650	1.2286
v42	903.2012	19.6512	892.1061	23.1828	895.6747	24.4840
v43	904.4287	18.9333	931.0508	6.1494	910.6978	4.2564
v44	921.7631	1.0634	979.2620	0.1730	976.5352	0.0762
v45	968.2954	0.3026	1000.4195	6.9666	996.0617	0.1364
v46	990.5214	0.1135	1004.3230	71.8270	998.4869	53.0474
v47	1014.4934	1.6915	1016.7654	30.2069	1014.0757	2.8880
v48	1025.5854	34.4312	1024.7631	63.5056	1023.2476	43.6592
v49	1029.4082	57.8754	1045.7853	5.6567	1043.6578	26.5381
v50	1037.2894	340.1805	1049.7504	90.6101	1052.6680	12.8470
v51	1049.0459	23.3239	1056.4932	75.5577	1058.6365	98.5499
v52	1061.0311	10.8809	1068.1684	201.9014	1067.8901	324.6731
v53	1076.8938	296.7205	1085.4880	7.9603	1085.7437	14.6607
v54	1098.9436	26.2930	1090.9627	297.6405	1102.4112	168.6807
v55	1107.0052	21.5504	1100.3391	14.1369	1105.1513	80.6428
v56	1114.4865	111.6968	1106.5341	15.7266	1107.6917	52.9012
v57	1124.8762	64.8779	1112.2270	17.9543	1113.1096	110.6474
v58	1136.2899	32.9446	1123.6900	147.9822	1124.3965	15.5233
v59	1143.9930	46.4980	1142.3304	19.7413	1147.4108	6.8195
v60	1153.5812	12.2622	1153.5851	5.1235	1156.2568	18.5305
v61	1187.3556	2.6133	1189.5762	1.1482	1188.7680	2.6817
v62	1202.9622	14.8319	1191.8071	17.4787	1207.1925	6.8880
v63	1221.3472	15.2850	1212.3826	38.4200	1209.5932	34.9284
v64	1228.5661	10.0262	1217.4393	54.8309	1232.1893	38.4335
v65	1243.1525	67.9179	1232.2866	46.5760	1238.9974	24.8158
v66	1260.1034	12.1883	1240.2356	103.8807	1254.4540	154.8546
v67	1269.2800	293.3669	1264.1253	32.2310	1259.6899	195.5711
v68	1274.3432	95.9223	1269.7183	15.6756	1282.2166	37.3602
v69	1311.4228	28.3517	1312.6594	20.6240	1306.4643	25.3847
v70	1332.8675	2.7356	1324.8820	39.6664	1322.1413	28.0517
v71	1344.4385	4.7474	1335.0938	0.3288	1346.0853	6.3099
v72	1354.4079	43.3598	1346.2010	1.4809	1354.0778	27.7143
v73	1364.8713	1.6898	1357.8982	0.3877	1355.7402	39.5714
v74	1369.5436	21.1788	1363.3407	43.4937	1367.3858	3.4110
v75	1371.4866	22.9781	1378.5267	18.4191	1377.0280	2.2367

v76	1397.7987	48.5276	1396.9055	31.6756	1400.7572	16.2309
v77	1407.0290	7.9464	1403.3751	14.4990	1425.3876	2.3011
v78	1421.0975	6.2608	1423.6320	14.8976	1426.9383	31.8187
v79	1434.0157	31.4377	1432.5538	42.1169	1435.6238	9.0780
v80	1441.5589	7.9180	1441.4885	0.9056	1440.3708	2.5945
v81	1459.0155	49.4913	1450.5775	16.3450	1450.5834	22.8667
v82	1471.7184	12.6740	1465.8928	11.8390	1479.5092	25.4907
v83	1498.2127	0.3961	1493.5380	2.0168	1498.3597	0.9475
v84	1516.9273	7.8890	1517.9451	2.1692	1513.7425	3.9603
v85	1536.4307	102.1085	1532.9670	63.5204	1535.7415	91.0935
v86	1639.2318	21.4688	1642.7628	10.7167	1639.3133	23.3770
v87	1653.0827	68.2439	1645.8845	29.6141	1651.9329	51.9275
v88	2575.9799	154.1253	2633.1665	106.8002	2641.2943	84.5341
v89	2797.8143	90.4396	2799.8677	109.4963	2791.8067	71.0351
v90	2990.1971	3.7208	2997.4697	5.0466	3002.5113	4.3599
v91	2996.8737	23.5375	3006.7194	13.7696	3010.1883	5.1470
v92	3008.9627	21.7404	3008.8013	11.9158	3012.6513	20.9083
v93	3031.5470	33.6057	3011.2777	2.5827	3019.3150	7.9814
v94	3054.0960	42.7552	3026.0651	33.0805	3034.0989	58.1964
v95	3058.3342	45.2278	3036.4174	109.8563	3049.4362	59.2764
v96	3141.3301	11.4205	3144.7762	10.6982	3125.8084	16.5074
v97	3182.5026	1.4163	3186.9836	0.5805	3187.7565	0.9077
v98	3190.9071	15.6172	3195.2743	8.3167	3195.5623	9.3940
v99	3206.3243	29.2585	3205.2356	19.8734	3207.7586	19.7894
v100	3215.7460	7.5241	3212.8436	13.0385	3215.0018	11.9069
v101	3231.5171	5.2232	3219.8786	2.9438	3229.2108	0.8055
v102	3544.0764	540.5107	3535.6910	552.7657	3582.4953	353.4124
v103	3720.6261	53.0595	3724.5077	49.1034	3727.6501	52.0538
v104	3729.1600	42.9986	3728.2698	57.6983	3739.6811	51.0664
v105	3729.4051	57.6982	3735.1745	40.0939	3749.1875	39.8312

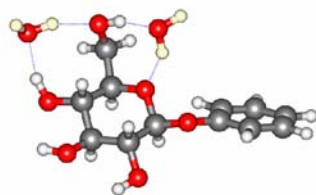
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	2.8670	0.0583	28.1003	0.1502	26.7935	0.0140
v2	31.5565	0.2547	33.5487	2.0735	43.9489	2.0229
v3	44.0916	1.9330	46.6110	0.1214	59.5324	0.4559
v4	51.9310	0.6958	48.7885	1.4944	61.3543	0.4878
v5	78.2598	1.2921	91.7689	3.5193	64.7231	2.6086
v6	87.7664	4.0733	99.9785	2.4584	91.1398	1.2433
v7	111.8786	4.4371	107.0168	1.1868	110.0889	7.7298
v8	131.8155	7.8259	131.0948	9.4726	115.8379	24.1720
v9	138.1010	1.9317	159.8103	1.5744	130.0894	41.3217
v10	158.7842	5.0169	172.7365	0.8145	150.9005	1.8491
v11	186.5439	77.3899	184.4829	1.0566	177.6703	1.1342
v12	207.8170	5.4487	201.4674	72.2727	198.5475	3.7044
v13	228.8838	44.2767	225.1162	5.6776	218.1974	1.8626
v14	233.8914	14.1917	247.2158	9.8400	236.8981	6.4597
v15	240.8590	6.6021	262.6542	40.6514	238.7681	6.4437
v16	250.0987	2.3864	276.9117	14.8171	261.5077	21.2402
v17	267.5977	8.4345	293.0469	17.6809	270.0065	105.5576
v18	311.5680	4.0810	308.3828	2.1758	298.2731	11.7383
v19	312.7698	11.9841	325.2856	16.3572	307.5960	14.1616
v20	363.4609	35.0901	356.9613	6.9254	341.6890	34.1699
v21	384.3826	63.7565	388.1156	87.1751	374.3210	101.5795
v22	401.9283	142.1166	404.5796	49.2695	397.5408	70.1754
v23	418.4816	46.2267	409.6057	75.3265	401.9178	87.7480
v24	424.5574	13.9726	425.2769	8.4645	405.6580	84.5243
v25	425.3559	76.2595	427.6539	59.0058	423.3571	2.7367
v26	432.3032	39.3462	441.9848	220.5929	425.2387	4.2984
v27	447.3263	39.0041	462.0253	32.8063	451.9785	80.8817
v28	456.3146	12.0760	479.2306	2.0265	480.9390	5.8071
v29	507.5794	38.6820	508.5274	9.5868	507.3671	4.1329
v30	535.2746	10.5214	519.3180	3.6648	521.2190	9.9357
v31	557.3288	7.5220	539.6050	8.1187	538.5500	12.7662
v32	571.9538	8.5171	596.0069	25.3325	580.0264	66.3424
v33	623.7153	6.3626	621.4969	3.9881	595.9459	52.7237
v34	636.7831	10.9407	639.7355	10.5947	621.4470	8.8653
v35	643.8778	14.8200	644.2852	10.3964	640.6084	22.5133
v36	705.9834	32.6468	651.7911	10.7846	646.7982	8.0734
v37	715.2216	11.0043	698.9750	16.5359	652.4006	13.9658
v38	764.9875	113.4168	765.0805	49.3155	701.6969	13.1556
v39	786.8912	49.9370	766.1582	126.1524	766.8081	70.8429
v40	841.0269	14.4425	833.6049	12.0454	834.0776	24.6098
v41	847.1816	0.2762	835.6568	17.7251	847.9743	0.4018
v42	910.3541	23.0745	894.8030	29.8559	899.8757	32.9060
v43	919.8602	14.4078	904.9052	3.8445	919.7420	4.6183
v44	931.9218	2.0444	970.3058	0.1773	978.6323	0.0245
v45	979.9920	0.2394	993.2792	0.0493	997.3050	43.6179
v46	1001.0730	2.1474	1005.7692	49.7366	998.7145	1.4690
v47	1015.2885	123.4576	1013.8953	1.1227	1012.5675	1.3679
v48	1022.1059	83.8550	1019.5851	7.4450	1022.6357	27.1971
v49	1029.3017	45.0259	1045.4256	2.8714	1044.7924	27.4865
v50	1045.3777	26.9353	1052.6487	113.1816	1047.1807	141.9504
v51	1049.5965	7.2689	1054.9802	62.9144	1053.8545	11.2162
v52	1066.5494	109.6446	1078.1700	129.4089	1069.8468	86.3868
v53	1078.6483	306.6659	1083.2223	10.5755	1085.9072	69.4103
v54	1099.5103	169.2394	1097.6025	337.8693	1092.2156	327.5603
v55	1100.8270	5.2718	1106.9420	72.5963	1104.8483	48.8358
v56	1107.3980	28.1093	1107.7556	55.1706	1109.0248	95.3679
v57	1110.3703	32.0827	1115.1502	163.6458	1115.0268	132.8238
v58	1125.3002	121.5200	1133.5263	12.7662	1126.3708	18.3774
v59	1142.2250	1.7432	1141.8059	27.4247	1146.1409	10.6889
v60	1143.5542	17.8037	1157.8677	6.3889	1159.8486	6.2677
v61	1189.4858	0.7035	1188.3919	2.2421	1186.7759	2.1477
v62	1193.3084	14.8267	1206.1700	10.5663	1210.3475	3.1332
v63	1212.7750	18.9806	1215.0570	31.1783	1213.0141	47.9167
v64	1216.0567	68.8604	1227.9145	22.5595	1229.8326	36.0492
v65	1236.1681	144.5945	1237.0021	17.0497	1235.2443	20.0226
v66	1245.9779	30.2539	1259.4605	340.8696	1249.0109	97.7518
v67	1258.6633	27.4724	1264.7583	37.9516	1259.0285	267.6067
v68	1269.1492	20.8763	1284.2172	20.8497	1267.4173	47.6330
v69	1313.6037	19.7760	1310.4072	26.9143	1310.1991	28.0158
v70	1335.3784	0.9065	1331.1226	32.6926	1336.2744	27.7309
v71	1337.6007	47.9580	1346.8042	2.1737	1347.5103	10.5917
v72	1341.7328	1.1431	1353.3518	13.6988	1353.8746	20.8154
v73	1358.1978	0.4092	1366.9352	7.2603	1354.9863	46.9040
v74	1363.4719	27.5743	1368.0369	34.7263	1369.7162	0.9796
v75	1387.0383	15.0829	1384.3764	14.0484	1376.3072	1.3651

v76	1396.3682	29.3301	1398.8150	14.8944	1389.0497	15.2078
v77	1398.5460	18.4472	1410.1300	9.9084	1414.5112	11.0868
v78	1424.6827	15.5766	1427.9550	3.4005	1427.1572	0.5674
v79	1430.9593	42.3865	1428.5168	31.1162	1434.6404	52.6375
v80	1441.8500	7.2662	1437.3252	42.4077	1438.0923	2.3962
v81	1450.0734	17.9213	1456.1290	27.5970	1445.2621	12.0447
v82	1464.0309	9.0538	1484.2007	18.0784	1456.6068	15.5777
v83	1493.4310	1.9150	1498.6801	0.5358	1498.4109	1.5703
v84	1514.4408	7.4449	1515.9792	2.2190	1516.8186	1.9767
v85	1533.3574	64.3911	1536.2317	95.9908	1536.2918	87.3113
v86	1642.4642	5.3083	1640.9761	25.4858	1640.6623	30.4611
v87	1645.5272	33.0711	1652.6808	57.8512	1651.5970	45.8587
v88	2630.7944	101.4886	2607.8120	134.9866	2580.0709	154.5401
v89	2799.1326	107.3439	2796.0975	103.1418	2793.2129	68.1813
v90	2994.7021	7.7329	2992.0898	17.9902	3004.7622	4.2340
v91	3004.2881	5.7872	2999.1061	2.0742	3014.4444	17.3827
v92	3011.3451	18.5464	3006.9780	7.8973	3019.9808	11.9348
v93	3025.9441	66.9660	3015.1411	9.6009	3035.2283	7.9486
v94	3031.9701	25.7156	3027.9354	95.5580	3045.5404	15.3979
v95	3049.4665	57.9708	3061.6478	35.0360	3051.0568	86.7815
v96	3140.2391	10.3764	3147.0955	10.0196	3155.8762	9.0049
v97	3186.3695	0.1611	3186.2667	1.4976	3183.8636	0.9142
v98	3195.5896	11.1251	3194.1723	9.4502	3193.8607	13.5066
v99	3206.2667	21.8638	3206.1847	22.0925	3204.7789	28.0046
v100	3213.9268	8.9287	3213.6606	14.7731	3211.8640	12.9724
v101	3231.3033	2.9904	3232.6897	2.6964	3229.2062	6.2347
v102	3545.6375	515.4246	3507.1261	660.7833	3722.2242	49.4015
v103	3723.1924	48.2694	3709.2612	56.4593	3727.9474	51.1287
v104	3735.3705	56.0192	3732.1629	47.4385	3739.5583	50.9854
v105	3738.4460	25.1224	3739.8067	33.2700	3745.2857	44.0593

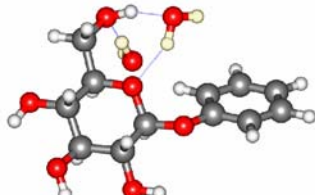
Table 5. β -PhGlc $\cdot$ (D₂O)₂

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

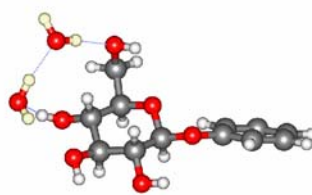
Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	0.00	0.00
B	10.11	2.96
C	2.58	5.09
D	1.18	6.54
E	9.44	7.24
F	???	???



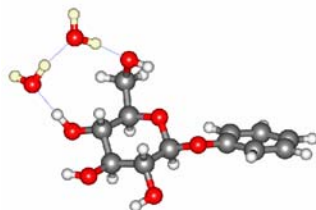
A



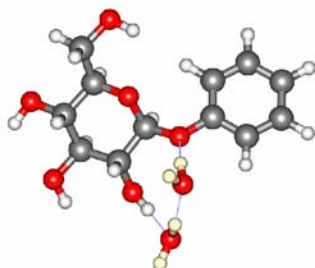
B



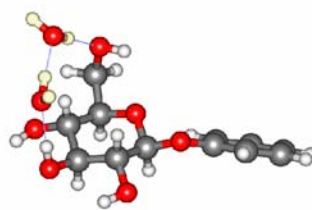
C



D



E



F

(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	-0.509997	0.791629	-0.150341
6	0.405570	1.882496	0.408797
6	1.746778	1.853581	-0.321701
6	2.381005	0.465775	-0.281829
6	1.384885	-0.543694	-0.881870
8	0.151900	-0.479692	-0.127778
8	-0.246120	3.131181	0.236348
8	2.576340	2.833771	0.293192
8	3.593687	0.535233	-1.014798
6	1.863615	-1.996167	-0.894635
8	2.398738	-2.465826	0.339021
1	0.405144	3.822819	0.442507
1	3.456048	2.749377	-0.113821
1	1.687440	-2.519082	1.019834
1	0.569300	1.674985	1.476890
1	1.580726	2.127876	-1.377094
1	2.576569	0.189497	0.762760
1	1.174291	-0.262953	-1.927354
1	4.231212	-0.105529	-0.622964
1	1.033614	-2.637783	-1.221245
1	2.668290	-2.082358	-1.630256
8	-1.628189	0.686908	0.677063
1	-0.810280	1.031791	-1.181576
6	-5.284033	-0.843049	-0.641325
6	-5.190092	-0.039158	0.500921
6	-3.956868	0.463901	0.912164
6	-2.804702	0.156297	0.180057
6	-2.880530	-0.655962	-0.955878
6	-4.127831	-1.144576	-1.362496
1	-6.247036	-1.230313	-0.962152
1	-6.082776	0.205604	1.070776
1	-3.866064	1.101455	1.786342
1	-1.985331	-0.925628	-1.504903
1	-4.185549	-1.774100	-2.246949
8	0.262929	-2.218351	2.070343
1	-0.101362	-1.523418	1.484399
1	-0.454076	-2.848629	2.234133
8	4.960375	-1.511682	0.260786
1	4.138223	-2.001899	0.497588
1	5.487558	-1.430482	1.068489

B			
6	0.207124	-0.890324	0.086242
6	1.330059	-1.903951	-0.152012
6	2.647636	-1.329977	0.361679
6	2.920183	0.051108	-0.235891
6	1.712895	0.969348	0.005726
8	0.540811	0.336912	-0.556883
8	1.108368	-3.123035	0.549345
8	3.757886	-2.158415	0.025157
8	4.062015	0.648057	0.365038
6	1.875198	2.342534	-0.642302
8	0.803922	3.231222	-0.331174
1	0.300515	-3.534330	0.201455
1	3.595900	-3.042471	0.393996
1	0.060896	3.042337	-0.949868
1	1.401296	-2.085149	-1.233870
1	2.581829	-1.228425	1.456592
1	3.075397	-0.060354	-1.320840
1	1.558178	1.100529	1.085750
1	4.781045	-0.005321	0.332882
1	2.794483	2.791965	-0.259212
1	1.972586	2.231322	-1.731044
8	-0.948984	-1.408491	-0.506921
1	0.050513	-0.716719	1.161199
6	-4.809490	-0.131078	0.461933
6	-3.718457	0.570583	0.976909
6	-2.403497	0.188374	0.679490
6	-2.198894	-0.925430	-0.140450
6	-3.282597	-1.637432	-0.666942
6	-4.583534	-1.237731	-0.364994
1	-5.823554	0.178511	0.699073
1	-3.873660	1.433751	1.618889
1	-1.584619	0.770651	1.089449
1	-3.089708	-2.493859	-1.306635
1	-5.421774	-1.794634	-0.775723
8	-0.405219	2.517640	2.083700
1	0.030309	2.926808	1.300398
1	-0.380963	3.182416	2.787194
8	-1.097452	2.137433	-2.041636
1	-2.025237	2.167413	-1.760701
1	-0.753964	1.288836	-1.698314

C			
6	-0.737801	0.588287	-0.186070
6	0.293215	1.636903	0.236771
6	1.557819	1.508100	-0.610126
6	2.080480	0.068698	-0.606612
6	0.958821	-0.939093	-0.903738
8	-0.183892	-0.713540	-0.058649
8	-0.196527	2.962969	0.059160
8	2.593852	2.346606	-0.093111
8	3.088022	-0.134137	-1.574151
6	1.393891	-2.377779	-0.644352
8	1.744135	-2.597548	0.729772
1	-0.964028	3.085406	0.641162
1	2.261039	3.259195	-0.089602
1	0.984686	-2.326289	1.273637
1	0.542358	1.455093	1.292161
1	1.328862	1.801202	-1.646036
1	2.461350	-0.133353	0.402766
1	0.665214	-0.848713	-1.962480
1	3.948775	0.107363	-1.153098
1	2.286674	-2.597519	-1.231694
1	0.589068	-3.065821	-0.933012
8	-1.824834	0.704700	0.689789
1	-1.066695	0.756279	-1.224798
6	-5.626675	-0.777438	-0.209443
6	-4.537280	-1.207758	-0.968231
6	-3.244526	-0.744971	-0.697032
6	-3.054524	0.172997	0.339937
6	-4.137688	0.606487	1.112252
6	-5.418009	0.128806	0.836438
1	-6.625394	-1.146521	-0.424899
1	-4.683300	-1.920499	-1.775933
1	-2.402354	-1.118600	-1.267582
1	-3.960891	1.313253	1.917865
1	-6.255910	0.470044	1.438862
8	4.174923	-1.591419	1.808721
1	4.777651	-2.308160	2.055146
1	3.372949	-2.019821	1.433364
8	5.107869	0.531086	0.160808
1	4.655239	1.342843	0.446625
1	4.889978	-0.154562	0.830069

D			
6	-0.827500	0.706587	-0.101751
6	0.066905	1.830449	0.425405
6	1.350659	1.891483	-0.398622
6	2.072203	0.544809	-0.428195
6	1.091205	-0.518706	-0.955536
8	-0.101679	-0.526571	-0.154370
8	-0.656612	3.048216	0.333232
8	2.160424	2.917451	0.165208
8	3.197335	0.669889	-1.284487
6	1.610696	-1.951325	-0.898348
8	1.741714	-2.412687	0.453070
1	-0.023929	3.766708	0.502274
1	3.007238	2.904963	-0.313361
1	0.930250	-2.151950	0.925082
1	0.314523	1.605654	1.473684
1	1.090808	2.161776	-1.436106
1	2.385565	0.281464	0.591085
1	0.847505	-0.280357	-2.003949
1	3.994854	0.295233	-0.841378
1	0.925294	-2.614181	-1.442072
1	2.600930	-2.012008	-1.355738
8	-1.886540	0.536227	0.786892
1	-1.203353	0.954551	-1.106823
6	-5.538059	-1.135578	-0.355972
6	-4.403922	-1.401775	-1.124755
6	-3.158646	-0.866220	-0.776027
6	-3.062036	-0.041975	0.349665
6	-4.191830	0.229320	1.129666
6	-5.423012	-0.320390	0.776265
1	-6.499666	-1.559505	-0.631762
1	-4.477357	-2.041428	-2.000872
1	-2.276967	-1.110549	-1.357516
1	-4.085910	0.875938	1.995457
1	-6.298130	-0.103638	1.383638
8	5.361642	-0.375830	0.064934
1	5.092307	-1.100392	0.679934
1	6.107425	-0.712560	-0.452277
8	4.212455	-2.282466	1.668899
1	4.511951	-3.150296	1.975111
1	3.306784	-2.403339	1.297808

E			
6	0.158925	0.055633	-0.322753
6	1.118606	1.255867	-0.349851
6	2.491747	0.762885	-0.814977
6	2.996150	-0.396415	0.038041
6	1.940787	-1.508417	0.060820
8	0.687110	-0.964506	0.516422
8	0.713972	2.264054	-1.251727
8	3.462821	1.802142	-0.750906
8	4.202326	-0.940521	-0.483849
6	2.281801	-2.648447	1.013669
8	1.274473	-3.651494	1.020936
1	0.150238	2.920764	-0.780157
1	3.096859	2.558380	-1.241598
1	0.444771	-3.227139	1.294210
1	1.204263	1.650904	0.673189
1	2.397702	0.414786	-1.856774
1	3.157705	-0.033938	1.066010
1	1.813666	-1.914931	-0.954742
1	4.805076	-0.197265	-0.654939
1	3.205101	-3.129739	0.685053
1	2.439275	-2.242306	2.024899
8	-1.075070	0.457351	0.221334
1	-0.000732	-0.329980	-1.340985
6	-4.639253	-1.503445	-0.747534
6	-3.432374	-2.196013	-0.860085
6	-2.218972	-1.576260	-0.541384
6	-2.229104	-0.243271	-0.123463
6	-3.428900	0.463514	-0.006168
6	-4.631151	-0.173046	-0.315051
1	-5.576956	-1.994352	-0.992389
1	-3.425571	-3.232309	-1.187807
1	-1.289642	-2.131316	-0.601572
1	-3.407902	1.500491	0.315055
1	-5.563378	0.378505	-0.226283
8	-0.729253	4.074966	0.277657
1	-0.356876	4.944264	0.483354
1	-0.951145	3.643999	1.134410
8	-1.341407	2.332514	2.329525
1	-1.220416	1.546410	1.756919
1	-0.931401	2.123213	3.181421

F			
6	0.605461	-0.506946	-0.343940
6	-0.500131	-1.536854	-0.109023
6	-1.681191	-1.243820	-1.042149
6	-2.161687	0.198088	-0.903916
6	-0.996203	1.183470	-1.040529
8	0.080855	0.814594	-0.168684
8	0.019606	-2.832735	-0.359536
8	-2.746401	-2.167663	-0.832966
8	-3.119927	0.526430	-1.906416
6	-1.377717	2.603201	-0.621662
8	-1.648783	2.678312	0.785706
1	-0.746632	-3.420697	-0.479970
1	-3.145732	-1.989144	0.050680
1	-0.860872	2.330992	1.240737
1	-0.820205	-1.444494	0.940336
1	-1.354821	-1.412989	-2.077047
1	-2.605154	0.322303	0.090424
1	-0.657900	1.195152	-2.089472
1	-3.753139	-0.210787	-1.949335
1	-2.288879	2.912801	-1.137262
1	-0.566758	3.298165	-0.873727
8	1.598642	-0.697413	0.613633
1	1.022771	-0.607492	-1.358478
6	5.546843	0.534598	0.039554
6	5.214551	-0.470812	0.955188
6	3.888250	-0.866587	1.120258
6	2.881997	-0.248802	0.369245
6	3.196958	0.766853	-0.539223
6	4.534547	1.145677	-0.702116
1	6.581767	0.838842	-0.090077
1	5.992767	-0.956316	1.538606
1	3.612766	-1.654603	1.814582
1	2.414302	1.275559	-1.090559
1	4.777839	1.935018	-1.409114
8	-3.732304	1.378555	2.163466
1	-4.538870	1.913937	2.191455
1	-3.067327	1.901183	1.657200
8	-3.857054	-1.365230	1.651171
1	-3.808719	-1.848869	2.488400
1	-3.854331	-0.405758	1.881511

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	23.4980	0.0588	24.5748	0.0284	23.9800	0.0606
v2	32.1572	0.9605	44.0791	1.3964	33.8045	0.7443
v3	37.2356	0.6333	50.6614	2.6123	38.7265	0.4543
v4	47.4886	4.0639	59.9940	0.7768	48.7321	1.2576
v5	58.1355	0.8145	64.6781	0.0344	54.0368	5.5719
v6	76.5218	2.4767	80.9990	3.7518	83.6805	2.7645
v7	91.3212	0.3504	89.8353	1.0971	89.6727	2.4082
v8	114.4864	3.7050	100.1943	3.2149	96.5174	2.8777
v9	133.2173	4.2136	113.5829	3.6754	110.7743	1.2415
v10	162.1411	7.9974	134.2139	66.8906	144.8511	49.6943
v11	163.8102	38.7202	135.1784	4.5564	150.9000	7.6267
v12	177.3057	15.0135	152.6538	5.3374	183.0810	7.4141
v13	192.8859	57.9758	183.1129	4.7770	201.3529	7.2058
v14	200.7329	40.5890	198.7894	5.4096	214.4221	13.5800
v15	206.8047	10.6395	214.0257	33.1429	223.2116	20.5807
v16	232.7930	8.4270	223.5547	20.7644	235.9329	4.5682
v17	242.8973	7.7671	238.8313	6.6238	244.0829	7.6123
v18	257.1210	24.2202	240.8340	2.9968	263.4243	4.2820
v19	263.8900	8.6409	246.7152	10.6992	270.6280	11.1538
v20	274.1287	0.6249	265.3523	25.4516	291.0770	13.2576
v21	294.3340	19.8142	294.0290	10.3288	302.8680	17.8473
v22	302.4487	22.6213	300.0429	5.5054	313.7552	3.3483
v23	308.8658	5.6549	312.7164	77.9479	327.9273	16.7295
v24	329.5226	2.1614	328.1263	9.7399	344.5172	20.6534
v25	355.4455	24.0591	351.4693	22.8784	363.2090	100.7978
v26	382.1547	99.1398	371.1010	106.9560	376.9129	103.4553
v27	414.8040	11.6227	394.5752	79.1560	394.8690	139.7295
v28	422.2986	3.6798	400.3402	29.1137	419.2711	9.1039
v29	427.3558	24.2785	408.0105	148.4861	421.4093	2.5876
v30	443.4411	74.7516	417.8079	66.4185	436.2586	95.4949
v31	457.4519	69.9549	425.9193	4.9670	448.8282	11.2802
v32	472.2098	14.7973	430.6098	4.4001	474.7119	63.8277
v33	513.7139	23.8024	477.6589	5.6138	514.5655	3.9423
v34	521.1197	55.4822	501.5364	12.5893	532.7293	68.7800
v35	534.7595	25.1188	522.7540	4.2580	536.3072	7.9599
v36	547.6328	46.1851	540.5388	14.1732	541.6048	55.7121
v37	579.4787	7.2782	545.8957	43.0650	575.6166	103.7125
v38	620.4588	5.5397	594.0086	30.3173	576.7799	73.1784
v39	635.0541	17.5984	619.7320	4.1448	621.9896	5.3908
v40	645.5478	15.3036	636.5428	15.4965	640.9878	8.5267
v41	700.1671	21.0827	645.0898	5.2590	653.2702	14.6333
v42	714.5399	1.8591	649.3001	23.6797	695.7183	18.3393
v43	766.5015	61.3811	695.4394	13.1560	714.3216	6.8227
v44	793.5819	54.8175	767.1097	83.4203	764.2076	70.7514
v45	810.1697	170.4730	828.9574	61.3256	832.7156	3.0540
v46	833.7528	26.3676	836.9546	94.3114	836.1631	16.9956
v47	838.1221	11.6204	856.1950	6.0420	841.0190	87.1720
v48	892.1313	19.6719	897.4718	31.3734	903.1899	3.6837
v49	906.5739	4.2500	926.9046	4.0176	909.2532	26.7975
v50	926.1572	3.5455	984.6623	0.0131	921.3282	2.7691
v51	971.9404	0.5593	997.0351	47.0153	968.9703	0.1068
v52	993.4062	0.1308	1005.1726	0.4993	992.3740	0.0970
v53	1014.3303	2.3516	1012.6807	3.6733	1014.4245	8.8582
v54	1025.9596	106.9970	1022.1655	51.0317	1022.8649	112.5999
v55	1027.4922	62.1993	1041.4137	55.6804	1032.6240	32.0838
v56	1033.6634	381.5650	1051.4399	57.6274	1046.5311	90.6157
v57	1050.8780	32.7139	1056.9346	222.0333	1053.9439	11.0243
v58	1071.0274	107.5799	1062.2282	61.0475	1062.7372	63.0629
v59	1076.8111	67.6281	1083.4273	126.9957	1084.2759	198.9417
v60	1100.1906	25.4483	1096.7444	123.4306	1095.0923	292.5577
v61	1107.1215	13.3214	1106.3291	45.4728	1106.9141	56.8403
v62	1114.9147	102.8515	1109.2013	106.4092	1109.8170	91.0529
v63	1125.8748	58.0670	1115.4801	86.8333	1119.6138	20.7532
v64	1139.1390	36.2464	1124.1479	13.0737	1134.4481	41.2712
v65	1144.9893	37.8997	1146.5442	8.3613	1143.1199	31.4708
v66	1158.4611	15.0555	1159.7080	14.3409	1147.4328	7.6915
v67	1188.0763	2.5567	1187.2501	2.5654	1188.3372	2.9074
v68	1203.0922	15.8098	1210.8373	12.1261	1204.4953	15.5037
v69	1222.9377	28.8156	1213.0096	31.1829	1213.8227	14.9917
v70	1223.5848	12.3707	1234.6265	34.9728	1237.1869	72.7882
v71	1240.4380	29.2668	1239.4758	56.4801	1241.0423	23.7123
v72	1261.3530	85.2352	1241.5993	26.9219	1247.4988	1.0353
v73	1265.7356	168.4494	1254.3691	191.6300	1255.8630	41.5867
v74	1268.5143	155.3353	1259.1956	180.1639	1260.6551	337.1592
v75	1284.0215	35.2468	1287.1586	29.1791	1289.8548	25.2612

v76	1315.5879	25.2112	1308.3097	24.2105	1305.0076	38.3520
v77	1337.1160	3.6888	1332.7422	28.3537	1340.3525	7.0007
v78	1343.9817	6.1780	1347.1747	10.6862	1348.8189	17.7618
v79	1352.6892	39.7027	1353.7550	41.0549	1357.4983	36.4367
v80	1364.5931	3.1624	1357.2516	30.2284	1366.4183	5.9851
v81	1370.6673	38.7916	1371.3542	0.2286	1371.8649	16.0814
v82	1391.5762	2.7126	1376.4123	2.4011	1373.1172	4.2630
v83	1398.5036	39.7336	1402.0575	12.7251	1399.1973	17.7281
v84	1407.6748	14.2592	1426.4081	0.7691	1411.3879	4.5587
v85	1422.0739	8.3343	1429.5136	36.6934	1425.2882	41.6634
v86	1442.2874	1.9322	1435.9811	3.5240	1429.5061	13.7569
v87	1459.9471	46.4069	1441.7200	2.6149	1433.3816	22.3937
v88	1476.6494	8.9209	1454.4435	19.6331	1446.3741	18.0234
v89	1483.0230	49.0717	1497.9557	2.3667	1493.0595	28.3186
v90	1497.6651	0.4701	1500.8465	22.3727	1499.0196	0.4027
v91	1512.1268	14.6053	1518.8771	11.6702	1512.4250	9.6932
v92	1535.9872	99.1022	1536.5208	82.6078	1536.0025	97.5170
v93	1639.4620	21.9695	1640.0181	29.4226	1640.9522	23.5934
v94	1652.6574	64.2790	1650.5786	40.2828	1652.8861	61.1054
v95	2524.7176	249.8494	2529.9931	222.4329	2548.5650	242.7325
v96	2616.7302	128.8491	2634.7765	89.9025	2577.8748	171.5167
v97	2791.0870	83.2630	2785.8235	67.8642	2752.3943	91.2234
v98	2795.1592	90.7876	2787.5033	63.8445	2789.6713	90.7789
v99	2989.1994	6.7668	3003.4473	4.3594	2999.1340	10.0744
v100	2998.9395	26.9773	3014.0996	23.7624	3005.4033	21.9158
v101	3020.0490	3.5510	3029.1001	3.6262	3021.6296	12.2669
v102	3033.6604	39.5632	3040.0020	15.7157	3039.9338	27.1434
v103	3043.3363	46.2038	3047.0490	19.6683	3056.9436	44.6287
v104	3054.9690	44.7686	3054.7163	62.6786	3061.9398	44.2465
v105	3123.7818	20.4844	3138.8439	13.8880	3159.6012	7.0498
v106	3184.1243	1.2214	3185.9320	0.4983	3185.3000	1.5988
v107	3192.4813	14.0704	3195.7224	13.0708	3192.8833	11.0267
v108	3207.4562	27.6030	3206.0906	25.3046	3206.1088	23.2589
v109	3217.2170	6.4710	3213.2157	10.4693	3213.5263	14.1081
v110	3225.9214	4.5429	3224.2665	16.3561	3235.0839	4.2151
v111	3463.0070	526.0554	3481.2442	500.4246	3421.8570	760.7598
v112	3478.0854	744.6292	3727.7091	53.3353	3725.8881	43.6999
v113	3716.7990	56.2469	3739.5544	51.8461	3740.3554	42.8061
v114	3727.8799	57.0999	3747.2132	41.5176	3745.7308	39.7514

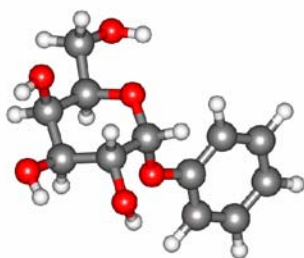
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	23.3604	0.0999	23.7326	0.9992	24.4191	0.3918
v2	25.2372	1.5437	29.6452	1.4857	33.4881	0.4199
v3	27.7457	1.1811	38.7381	2.0733	38.6182	0.2729
v4	38.9288	0.3972	45.2613	0.2578	42.4352	0.7062
v5	45.0971	0.3331	47.8408	0.2848	54.5673	0.3842
v6	67.1061	3.8952	60.0540	1.1040	76.6489	4.8658
v7	89.1621	2.4294	90.7851	0.7159	89.3881	1.4896
v8	95.0871	3.0415	103.7712	3.6590	96.2727	11.1227
v9	112.3615	6.1780	118.3693	1.2689	109.6835	10.8825
v10	140.0778	2.9075	135.9263	18.8459	126.6642	41.3330
v11	149.0407	57.4863	145.0838	10.5794	140.4149	4.7030
v12	166.1815	26.8767	162.2803	44.3373	155.6447	62.3239
v13	199.6002	54.7511	168.1224	2.5885	186.4738	16.4276
v14	206.7273	4.5656	180.4093	14.8286	205.0504	5.0187
v15	211.8609	7.4123	188.1136	38.5529	208.8830	32.8366
v16	235.5500	10.0609	212.4838	3.4707	237.2782	18.4357
v17	242.9314	1.6306	237.5164	10.7209	243.8597	3.4597
v18	256.0349	7.3066	238.8059	5.8173	248.3972	6.7710
v19	261.6304	24.1243	251.7389	76.0513	255.8824	15.1592
v20	270.2090	15.1054	270.7999	5.9090	262.9593	1.7037
v21	292.2287	4.3382	271.9605	23.2488	291.8269	2.1075
v22	303.8282	5.8734	302.1743	19.6236	296.3998	12.6365
v23	312.4774	40.4847	318.7045	4.2332	311.6144	39.2085
v24	332.0620	12.0648	347.2525	15.2204	325.7255	5.2470
v25	371.0029	63.8766	378.9891	66.5306	341.8688	11.6615
v26	389.8086	82.7646	398.8703	44.9778	387.3917	47.7409
v27	405.9426	33.7574	407.6317	7.3901	418.2883	7.9281
v28	421.8359	0.5187	418.0475	135.3439	422.1344	1.4687
v29	426.4535	63.0627	420.3255	3.6932	428.5645	136.5422
v30	441.7764	27.7046	428.4791	78.7485	440.2858	4.6972
v31	451.4113	55.6123	438.2378	115.4650	455.7331	16.8280
v32	477.0927	76.6836	451.8702	23.1595	499.9650	154.5993
v33	514.2951	7.4064	479.7659	10.0231	514.5696	3.5362
v34	531.1802	31.1610	499.7871	12.8824	534.1014	5.5134
v35	534.6899	10.6678	524.3990	10.4934	542.2085	4.3451
v36	552.7820	35.1143	544.4448	42.3354	560.8175	20.3148
v37	571.7537	4.9610	550.2701	23.6663	578.5077	11.5171
v38	617.7014	20.3619	593.7974	22.5556	588.7946	116.1276
v39	624.5546	30.6293	621.1119	3.6025	622.7610	6.4011
v40	635.3903	8.7579	634.4853	9.1269	638.4647	0.9766
v41	650.7344	38.3561	648.5264	6.2887	653.3775	23.0981
v42	697.4995	22.7193	654.1485	23.1502	697.8328	22.7750
v43	717.5704	0.4587	705.0428	21.4632	723.1080	4.7470
v44	761.5455	113.3910	765.7831	106.3716	765.4368	63.6123
v45	765.8581	63.1533	771.6179	78.6399	814.7589	131.2747
v46	834.0742	6.5996	835.9355	23.9487	834.9974	5.3286
v47	838.8423	17.3325	843.0012	3.6588	839.3359	11.7371
v48	904.6696	2.8178	892.5469	23.7940	905.3623	3.2902
v49	916.8580	5.9139	915.2858	4.1386	909.0940	20.2382
v50	919.6188	41.2829	975.8420	0.3294	925.3315	37.3741
v51	969.7755	0.3863	997.2563	0.1186	969.3464	0.3048
v52	991.4032	0.1008	1004.9661	62.3075	990.7742	0.1410
v53	1014.5635	1.4471	1015.0623	5.8604	1010.1087	75.6614
v54	1025.2134	35.0444	1026.9686	80.2373	1015.6914	11.5067
v55	1031.4354	83.5433	1049.0334	23.0062	1033.8756	336.8000
v56	1037.4302	290.3363	1051.1474	46.2085	1039.2913	10.0529
v57	1049.3802	35.1949	1058.1931	155.7554	1050.9983	15.5273
v58	1060.2708	18.5068	1067.1907	152.6971	1055.6133	10.0107
v59	1080.1146	335.1078	1084.2029	4.9119	1082.3399	159.0932
v60	1102.6113	34.0662	1092.5854	335.5368	1095.3332	271.1149
v61	1106.7592	11.7527	1108.5347	11.7395	1106.0224	7.5601
v62	1114.0128	147.4456	1109.9495	5.2086	1110.8689	24.7242
v63	1122.2249	39.2247	1119.3486	10.1903	1123.0091	72.9829
v64	1133.2096	33.4479	1127.4713	145.4788	1137.6535	51.5043
v65	1141.8912	34.0877	1144.5880	27.1006	1149.7545	13.2115
v66	1153.2093	8.8450	1157.0585	8.0451	1150.6324	4.9420
v67	1187.5266	2.3220	1190.3181	0.9789	1187.4854	2.2972
v68	1201.8625	13.8817	1206.3575	13.7466	1202.9401	14.6187
v69	1223.1124	20.8848	1213.0698	39.6120	1226.1060	39.7343
v70	1235.7188	24.3682	1228.6239	28.9171	1245.9863	14.3430
v71	1244.2835	29.4393	1236.6073	41.6014	1248.8997	41.9247
v72	1254.2481	32.0766	1247.5810	264.6637	1256.2570	35.5105
v73	1261.3275	18.2295	1250.8779	35.8604	1264.7955	139.5261
v74	1268.9052	226.8435	1264.7835	33.3853	1270.7522	238.3637
v75	1274.4563	159.3389	1275.4752	13.2198	1286.5092	44.8928

v76	1316.3941	29.6491	1314.7719	13.2687	1308.3133	28.5349
v77	1330.8222	6.5683	1326.0110	44.9866	1326.2953	1.0002
v78	1343.6752	4.2327	1344.6025	1.8341	1338.5482	23.5390
v79	1354.1299	33.5950	1352.6217	2.2945	1344.0216	0.3159
v80	1363.0840	5.8762	1362.6567	32.4996	1362.3102	13.4048
v81	1367.8055	10.4454	1368.3331	3.8799	1367.6649	20.9288
v82	1370.4135	33.2354	1381.7182	15.2560	1387.3589	3.4540
v83	1397.3109	44.6843	1401.4961	18.4441	1391.0969	40.6358
v84	1408.3209	5.2559	1406.3265	25.3260	1403.8167	5.3256
v85	1420.5386	8.7396	1429.9923	24.2592	1419.9818	1.1366
v86	1437.6910	32.4509	1430.6192	38.3287	1436.3061	50.4615
v87	1441.8073	21.1987	1441.9262	1.2436	1449.6978	6.2606
v88	1460.5597	47.6828	1449.6100	16.5977	1462.5680	57.4187
v99	1493.3465	17.7416	1480.9765	15.0030	1484.4432	36.4838
v90	1497.6341	0.3201	1499.1795	0.7912	1498.0490	0.4015
v91	1519.1586	7.2511	1515.8016	2.1412	1515.5852	7.1467
v92	1536.2422	102.4461	1536.4736	93.0091	1536.4304	100.9522
v93	1639.3227	21.5830	1642.8170	25.0438	1639.4928	21.1750
v94	1652.9166	68.4799	1651.6511	48.2928	1652.9837	67.7494
v95	2493.5721	300.6653	2543.5226	209.5736	2507.1089	348.1744
v96	2536.0420	372.4375	2605.5928	209.8704	2543.8355	231.6131
v97	2788.2664	63.7226	2794.3839	73.0684	2785.4917	88.0482
v98	2793.6336	94.5495	2794.4642	102.1598	2789.0890	61.4024
v99	2988.2690	11.3834	2995.0902	4.9025	3006.5041	6.2458
v100	3003.3946	16.6236	3003.9828	11.8965	3009.2909	17.3576
v101	3012.9695	16.4338	3010.7418	11.2303	3021.2469	33.3756
v102	3032.1351	37.3744	3021.9165	0.4579	3053.7917	28.4785
v103	3053.0814	16.0380	3025.9512	50.4558	3057.9610	52.4572
v104	3054.2682	73.4285	3038.9922	99.3544	3089.7359	29.8179
v105	3139.9925	14.8422	3146.5983	10.2434	3151.8732	9.0846
v106	3182.3774	1.3738	3187.2092	0.3127	3182.7503	1.2827
v107	3190.8481	15.7719	3195.9928	13.1091	3191.1415	15.6817
v108	3206.3132	30.2331	3209.1833	23.9869	3206.5461	29.7140
v109	3216.7007	6.8749	3218.0225	4.6180	3216.5764	6.8587
v110	3227.0989	4.8826	3229.9033	1.7613	3229.0314	4.8563
v111	3445.7770	1002.7995	3469.9460	757.3794	3482.2787	466.0319
v112	3703.1169	72.9474	3718.1457	49.3768	3704.1775	41.7619
v113	3720.5071	52.4442	3727.7071	55.3608	3711.0740	57.5404
v114	3727.4003	56.5846	3740.6923	30.9599	3717.0316	54.5822

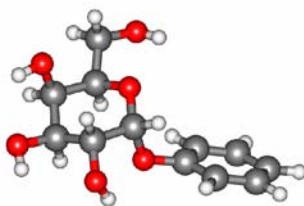
Table 6. α -PhGal

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

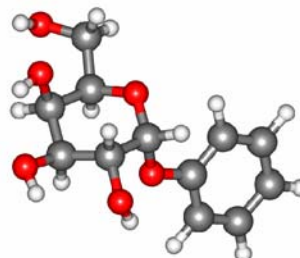
Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	0.00	0.00
B	3.26	1.95
C	1.83	2.09
D	1.01	2.98
E	0.97	3.07
F	5.21	4.82



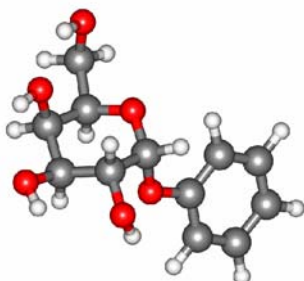
A



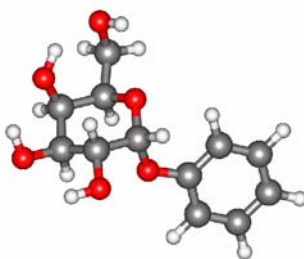
B



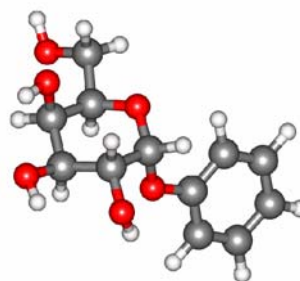
C



D



E



F

(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.200914	-0.467667	-0.846837
6	1.404727	-1.410910	-0.720388
6	2.192682	-1.119864	0.560107
6	2.586753	0.360854	0.627249
6	1.341635	1.232800	0.443839
8	0.593049	0.874504	-0.743156
8	1.024256	-2.782552	-0.786645
8	3.396771	-1.884100	0.596645
8	3.546718	0.675165	-0.373601
6	1.653777	2.718585	0.299261
8	0.470491	3.509383	0.310472
1	0.261403	-2.901653	-0.193652
1	3.180507	-2.787850	0.308837
1	-0.083417	3.218680	-0.431678
1	-0.273053	-0.569775	-1.828064
1	2.053867	-1.236326	-1.582386
1	1.570179	-1.360997	1.434702
1	3.002776	0.570536	1.626276
1	0.690773	1.092565	1.317573
1	4.222849	-0.023977	-0.340617
1	2.237076	2.882685	-0.614589
1	2.249701	3.049520	1.155071
8	-0.717933	-0.866460	0.169526
6	-4.769226	0.155151	0.080889
6	-3.894287	0.784124	-0.805562
6	-2.527924	0.479741	-0.806157
6	-2.044393	-0.480370	0.088477
6	-2.912309	-1.114380	0.985166
6	-4.268841	-0.793788	0.979628
1	-5.826744	0.403457	0.077054
1	-4.267668	1.530687	-1.501844
1	-1.857922	1.000888	-1.480156
1	-2.511067	-1.851319	1.675110
1	-4.937112	-1.290294	1.678420

B			
6	0.163934	-0.603687	-0.685121
6	1.379852	-1.513789	-0.463266
6	2.251635	-0.996969	0.685019
6	2.633399	0.470769	0.458664
6	1.363971	1.291689	0.222763
8	0.541319	0.737284	-0.829293
8	0.996020	-2.868683	-0.242133
8	3.463679	-1.744263	0.775167
8	3.509380	0.603499	-0.653142
6	1.624516	2.737273	-0.186512
8	0.414083	3.484942	-0.246556
1	0.279517	-2.857080	0.417644
1	3.236843	-2.685624	0.682481
1	-0.162077	3.049584	-0.896075
1	-0.361907	-0.861723	-1.609291
1	1.971127	-1.513329	-1.382747
1	1.692955	-1.075205	1.629946
1	3.121262	0.853633	1.370029
1	0.782643	1.290072	1.155190
1	4.197578	-0.076561	-0.549129
1	2.249515	3.224843	0.567736
1	2.155365	2.757946	-1.145794
8	-0.706363	-0.819481	0.433722
6	-4.745230	0.178343	0.020780
6	-4.239175	-0.960275	-0.613806
6	-2.887461	-1.293197	-0.491738
6	-2.044652	-0.473098	0.263219
6	-2.537967	0.665817	0.901026
6	-3.892915	0.986619	0.778872
1	-5.797569	0.432233	-0.072929
1	-4.897489	-1.597503	-1.198598
1	-2.488407	-2.185448	-0.967185
1	-1.864302	1.287600	1.482517
1	-4.279437	1.873192	1.274692

C			
6	-0.023082	-0.505885	-0.868817
6	1.081676	-1.557771	-0.712409
6	1.915085	-1.274458	0.539484
6	2.455595	0.159006	0.535648
6	1.328757	1.160815	0.257324
8	0.509969	0.789022	-0.871645
8	0.566732	-2.886489	-0.691467
8	3.040290	-2.150474	0.609693
8	3.481638	0.319227	-0.444270
6	1.860146	2.561689	-0.092581
8	2.880820	2.990337	0.798656
1	-0.193151	-2.893502	-0.082891
1	2.731389	-3.044486	0.382497
1	3.693437	2.518179	0.551671
1	-0.542679	-0.618412	-1.825844
1	1.725842	-1.498068	-1.593944
1	1.283645	-1.406431	1.430447
1	2.862968	0.381086	1.532622
1	0.697257	1.209323	1.154398
1	4.053479	-0.466190	-0.380617
1	2.214207	2.547005	-1.129777
1	1.047685	3.289024	-0.014444
8	-0.942386	-0.743390	0.197917
6	-4.870097	0.681768	0.125874
6	-3.934264	1.231574	-0.751426
6	-2.605822	0.790141	-0.757396
6	-2.225115	-0.228505	0.122460
6	-3.153458	-0.783396	1.011044
6	-4.470362	-0.325826	1.011015
1	-5.897173	1.035704	0.125152
1	-4.228674	2.022687	-1.436341
1	-1.881424	1.253201	-1.417435
1	-2.830859	-1.567994	1.689697
1	-5.186804	-0.761899	1.702426

D			
6	0.056517	-0.372408	-0.824159
6	1.171746	-1.424975	-0.777487
6	1.953906	-1.322311	0.534798
6	2.457576	0.106870	0.757410
6	1.299799	1.105697	0.620257
8	0.555515	0.914992	-0.596199
8	0.678519	-2.747248	-0.972757
8	3.098273	-2.175019	0.514596
8	3.488393	0.422251	-0.180901
6	1.734489	2.574647	0.673270
8	2.515598	3.011869	-0.420102
1	-0.114215	-2.844806	-0.416013
1	2.822431	-3.030345	0.142194
1	3.198755	2.338688	-0.587151
1	-0.413202	-0.340798	-1.812328
1	1.849024	-1.228364	-1.612793
1	1.296853	-1.598642	1.372506
1	2.858115	0.189293	1.779797
1	0.629771	0.935115	1.477192
1	4.095795	-0.338352	-0.204322
1	2.261250	2.725956	1.631457
1	0.838803	3.203397	0.682432
8	-0.909425	-0.788348	0.145036
6	-4.857493	0.580187	0.089971
6	-3.888952	1.277199	-0.634040
6	-2.552996	0.859146	-0.638860
6	-2.197992	-0.284722	0.083795
6	-3.159210	-0.988873	0.818305
6	-4.483655	-0.553356	0.820605
1	-5.890412	0.916735	0.089934
1	-4.163771	2.165456	-1.197131
1	-1.804339	1.431868	-1.173955
1	-2.856189	-1.870379	1.376398
1	-5.226066	-1.105408	1.391212

E			
6	0.042147	-0.383277	-0.812922
6	1.189216	-1.397650	-0.792182
6	1.950116	-1.330575	0.539050
6	2.432145	0.103042	0.802561
6	1.263275	1.093293	0.643047
8	0.568379	0.922713	-0.606143
8	0.675138	-2.693494	-1.040952
8	3.038795	-2.251441	0.522222
8	3.520780	0.328794	-0.094368
6	1.679478	2.561961	0.683155
8	2.557549	2.906250	-0.397152
1	1.394134	-3.320209	-0.849910
1	3.770182	-1.811033	0.051572
1	2.061671	2.778106	-1.223601
1	-0.442198	-0.353720	-1.793597
1	1.875270	-1.097617	-1.597800
1	1.288105	-1.658932	1.345975
1	2.795569	0.176947	1.840387
1	0.563258	0.915120	1.472542
1	3.564116	1.282157	-0.306610
1	0.785477	3.197848	0.663908
1	2.235180	2.770823	1.601991
8	-0.889951	-0.737740	0.183560
6	-4.874652	0.507989	0.085254
6	-3.931222	1.203331	-0.672344
6	-2.583336	0.824570	-0.666189
6	-2.188671	-0.277939	0.099934
6	-3.126862	-0.981536	0.865000
6	-4.462892	-0.584960	0.857297
1	-5.917486	0.812633	0.077145
1	-4.236080	2.058447	-1.270622
1	-1.855718	1.394336	-1.233172
1	-2.792495	-1.836978	1.444324
1	-5.186955	-1.138082	1.450164

F			
6	0.027907	-0.567969	-0.859998
6	1.149782	-1.592432	-0.642293
6	2.005099	-1.210673	0.569215
6	2.521442	0.225493	0.430865
6	1.340060	1.167981	0.177017
8	0.529921	0.737901	-0.936123
8	0.648718	-2.921559	-0.521168
8	3.141287	-2.068566	0.674190
8	3.447655	0.323206	-0.646557
6	1.764334	2.595844	-0.151100
8	2.340699	3.143038	1.036987
1	-0.099942	-2.892219	0.100309
1	2.836368	-2.979228	0.519842
1	2.887792	3.905777	0.800689
1	-0.490277	-0.745991	-1.807676
1	1.780366	-1.588193	-1.535025
1	1.397767	-1.283271	1.483943
1	3.001919	0.532760	1.370511
1	0.720988	1.188157	1.084385
1	4.078263	-0.409274	-0.537514
1	0.874823	3.164955	-0.453048
1	2.482293	2.582603	-0.978220
8	-0.887245	-0.758306	0.221161
6	-4.842473	0.582208	0.079944
6	-4.417605	-0.356078	1.027421
6	-3.091857	-0.786374	1.048941
6	-2.178958	-0.273959	0.119398
6	-2.585403	0.675914	-0.823890
6	-3.922428	1.090518	-0.838158
1	-5.876423	0.915188	0.062692
1	-5.121264	-0.759135	1.751278
1	-2.749540	-1.517070	1.776356
1	-1.874364	1.108171	-1.518322
1	-4.236452	1.828227	-1.572289

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	29.7502	0.1134	26.4024	0.0756	26.9997	0.1920
v2	47.3551	0.0349	30.7479	0.2748	41.3960	0.1692
v3	51.6527	0.6837	52.4423	0.7802	56.6081	2.6384
v4	98.2544	4.5277	96.2519	0.9903	75.8230	1.8606
v5	113.2869	0.1769	102.0618	3.9213	110.9690	6.5056
v6	130.5447	4.1585	127.1614	0.2067	123.6377	2.6496
v7	140.0300	0.8256	131.5257	3.7743	140.1195	0.7415
v8	166.4857	2.4188	166.4136	1.6108	179.2543	0.4391
v9	197.2523	0.7587	187.7068	2.7892	192.2404	3.5301
v10	242.9602	11.9384	232.4969	3.9998	231.6386	8.7385
v11	248.9016	1.0345	253.2702	4.8505	253.6813	2.8928
v12	269.5953	8.4772	268.5674	9.9833	268.5274	5.2985
v13	279.3936	1.3999	305.9661	0.3074	287.7779	5.0577
v14	334.1973	32.0147	335.4179	14.9326	318.8274	1.4483
v15	358.8583	11.1570	368.5221	15.8608	359.2075	9.2301
v16	367.0182	66.9258	386.4705	5.1144	392.8392	36.9798
v17	386.0596	53.4101	406.0168	30.5548	406.1756	14.0974
v18	400.7787	70.2473	416.9955	157.6673	420.9684	5.8232
v19	423.0336	1.8223	425.4125	22.6070	422.3175	0.3707
v20	425.3621	13.3777	436.6948	22.0238	475.6700	156.5698
v21	452.6803	120.3148	454.5194	129.5584	482.0003	44.7557
v22	475.0154	20.6682	469.1879	19.8710	492.1589	214.7940
v23	494.8216	174.2543	477.0791	22.1414	506.8994	45.1820
v24	519.3809	10.2743	514.0313	151.4686	516.6902	6.0701
v25	535.1237	9.3919	548.2930	16.5876	529.9117	14.8001
v26	553.3976	12.0173	553.8113	7.5628	559.4414	22.7711
v27	627.2821	0.3843	628.2995	1.2399	626.3600	1.3661
v28	670.2673	11.5488	656.0851	19.6594	644.0377	19.0412
v29	689.2819	61.3895	688.3282	53.8618	672.2663	38.1364
v30	701.1771	21.2815	701.5155	29.5540	700.0596	21.1675
v31	710.3401	2.9966	713.4484	7.0664	710.1184	3.7993
v32	764.7870	71.0131	760.7988	33.0583	759.0189	34.3990
v33	774.7159	24.1255	790.1771	48.1451	766.9578	47.7688
v34	812.0076	10.9061	813.1173	12.0071	804.4294	3.2105
v35	835.2504	0.8465	844.3125	0.2308	836.3517	0.1601
v36	861.3597	73.8495	863.8209	51.0449	865.3921	78.9304
v37	894.0364	10.8127	892.7420	31.4596	905.5046	15.0848
v38	905.1611	9.2292	914.8180	31.2780	908.1292	0.9973
v39	930.3262	20.1891	932.9021	13.6023	959.3464	80.0391
v40	970.5178	0.0342	975.1012	48.8370	971.1396	2.3301
v41	982.2662	52.7735	976.7782	30.8805	977.7177	29.2707
v42	993.1155	0.2369	998.8450	0.4310	993.0619	0.2202
v43	1011.0103	22.4515	1007.7636	31.7829	1002.9495	29.7568
v44	1014.6870	0.9664	1018.3960	1.3528	1014.6178	2.9971
v45	1042.8431	164.3123	1039.5999	161.6447	1033.2483	158.5931
v46	1054.0808	66.0800	1048.0154	14.1363	1052.4149	38.1956
v47	1073.1346	126.4665	1070.6413	113.9103	1086.7881	133.6259
v48	1091.7851	75.1338	1091.0732	131.7205	1095.5866	288.5812
v49	1096.1887	173.3060	1095.6218	102.1843	1097.3945	83.2712
v50	1111.2155	15.7621	1103.0116	4.6853	1103.3326	5.7381
v51	1125.1802	218.2405	1127.8617	213.8050	1110.8361	15.0703
v52	1134.4986	7.1299	1135.5402	9.1986	1131.0905	162.9798
v53	1138.4162	9.0802	1139.8878	13.9631	1141.3950	0.8455
v54	1149.4038	55.2578	1151.3987	61.4087	1151.9408	56.0743
v55	1188.4758	3.5197	1189.2700	0.0456	1188.3086	3.1368
v56	1207.8355	17.9839	1194.9996	16.7141	1203.6390	17.1398
v57	1221.7266	25.8438	1223.3184	22.3403	1205.5280	16.1570
v58	1230.8120	29.4480	1231.5772	40.2145	1231.9941	37.8099
v59	1251.1733	296.6311	1241.5198	189.4601	1251.1105	287.7888
v60	1260.9516	10.7009	1258.8028	11.9346	1260.3706	38.8317
v61	1267.0887	67.0235	1268.1189	66.5047	1275.9346	71.1113
v62	1307.7090	31.6002	1310.1266	37.3459	1316.5532	6.6671
v63	1322.4716	4.6016	1326.8178	3.1448	1336.8523	20.2450
v64	1348.1647	5.4175	1335.3498	0.4280	1346.8745	4.5533
v65	1365.9796	1.5005	1358.4004	3.8114	1362.8674	6.1139
v66	1368.2103	9.5991	1363.0408	34.1431	1366.5182	8.0756
v67	1375.7724	21.7554	1368.0215	6.8628	1375.4520	24.5034
v68	1390.4433	47.4108	1391.8750	30.6506	1394.1412	26.5677
v69	1392.7740	22.7781	1393.5644	16.5852	1399.6378	20.6643
v70	1399.7829	16.9101	1401.9589	5.5835	1405.2538	19.6012
v71	1401.8058	12.6774	1404.5997	23.6499	1411.7704	15.1154
v72	1431.2647	7.9438	1431.9464	7.6603	1425.2408	27.8487
v73	1433.7419	20.4661	1435.4322	27.2878	1433.3089	10.7672
v74	1445.2074	13.3760	1443.6952	14.9451	1438.4285	9.3304
v75	1449.6342	26.3739	1450.9665	19.8935	1449.3592	22.2914

v76	1498.5459	0.6598	1493.2171	1.3836	1498.5841	0.6153
v77	1514.7137	2.2563	1516.3198	2.0176	1523.6445	2.4300
v78	1536.9952	96.6230	1534.4149	72.3436	1535.6568	98.1441
v79	1640.5709	23.7492	1641.2016	8.0980	1639.4133	23.5057
v80	1652.5259	63.4936	1646.9023	42.2286	1652.0596	61.7087
v81	2996.7542	35.5055	2996.4675	35.7748	3021.7726	16.7758
v82	3024.8089	27.5051	3023.4018	24.9244	3031.9953	21.6716
v83	3049.3725	21.2107	3044.3780	27.7420	3052.4059	30.2904
v84	3066.9203	32.6066	3066.2256	33.0716	3068.8696	36.0965
v85	3096.4977	19.6688	3099.7076	17.1682	3093.5429	19.5177
v86	3120.7846	10.4098	3119.3572	11.3009	3117.3981	11.8053
v87	3123.6765	23.2787	3122.9999	24.2217	3129.5283	26.3908
v88	3185.4959	1.7905	3184.6621	2.0741	3184.9344	1.6143
v89	3192.9331	9.4327	3192.7393	5.1664	3192.6526	10.3324
v90	3204.7292	22.7606	3201.3328	21.0210	3204.3129	23.7784
v91	3212.9068	15.6792	3210.0799	20.1092	3212.3829	14.9469
v92	3231.8620	3.3927	3218.4417	3.4881	3234.0846	0.9642
v93	3707.6732	46.2094	3698.6950	47.4625	3703.9307	75.9916
v94	3709.7222	64.6907	3711.1517	61.7383	3706.6433	46.6579
v95	3716.5654	45.8792	3717.6767	46.1667	3717.3636	48.2436
v96	3749.0014	25.9444	3739.6645	28.5746	3728.7735	34.8539

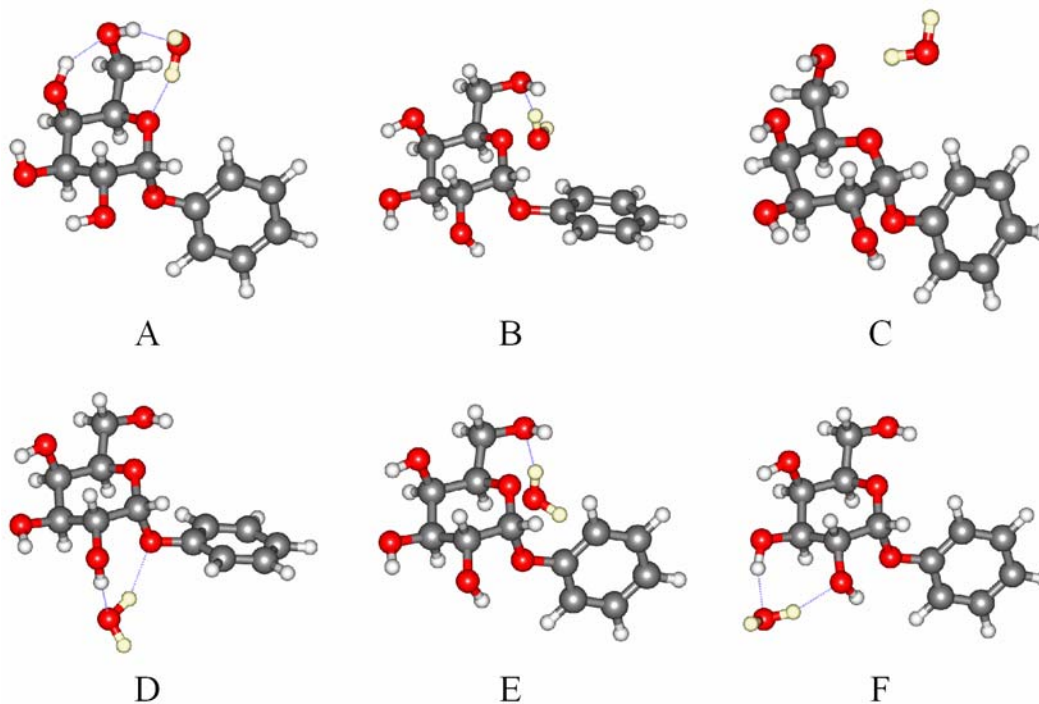
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	31.1049	0.0434	29.8946	0.1039	28.8982	0.0406
v2	43.7359	0.1947	46.3786	0.1330	44.2626	0.0072
v3	55.7661	1.2437	55.5518	0.3458	59.1070	1.1360
v4	95.9720	2.3048	88.7897	2.7269	84.5603	0.4521
v5	117.4139	5.4962	120.6106	7.0323	111.9582	11.8810
v6	135.7430	0.3519	137.0614	11.7054	129.8348	1.1001
v7	140.1458	2.1819	141.1484	0.7444	142.4773	3.3555
v8	190.7611	1.6884	191.3828	2.3007	170.8655	115.4342
v9	211.1732	6.0368	215.1176	0.4874	182.7325	1.7259
v10	252.7957	2.6337	254.3248	4.0709	208.3691	5.6674
v11	263.0477	5.1586	270.7086	3.6840	224.7284	5.7872
v12	269.9705	5.1095	274.4985	15.2293	255.6824	3.3442
v13	294.0266	1.5605	297.0427	7.8682	267.5444	6.5374
v14	317.1925	6.7686	330.3449	3.7135	281.6107	7.4422
v15	353.8786	6.4703	358.8670	13.6926	328.6664	5.5471
v16	380.0148	14.2713	374.0129	19.8220	356.9776	6.9144
v17	401.4786	35.9954	381.5201	35.9235	395.7072	40.8138
v18	421.9201	0.2842	401.6875	124.4458	410.1446	19.8057
v19	427.2054	14.7743	423.2189	0.0211	419.5677	28.1480
v20	467.4593	176.1962	436.9667	33.6475	422.9220	2.0660
v21	491.2884	158.5740	497.5259	9.5882	447.3445	93.9528
v22	495.6760	28.4079	515.8757	31.5604	491.2615	58.2696
v23	505.6238	65.2348	523.3263	139.2660	496.9884	147.7497
v24	519.7354	12.1860	537.5275	2.4234	517.9740	6.2571
v25	537.6180	30.9158	572.7306	14.6068	531.0942	12.2481
v26	572.6655	33.8305	626.4604	1.0281	556.1307	12.7738
v27	626.5577	4.0087	644.1917	65.9289	626.3440	1.6410
v28	654.5560	3.5962	669.3014	74.3410	644.5594	18.2062
v29	700.3765	18.7298	700.2744	24.8404	675.8011	44.0591
v30	707.2868	16.7282	708.9074	4.6767	700.1909	21.2434
v31	750.0325	10.0993	757.8270	9.2925	709.3743	4.0052
v32	762.4824	79.5716	766.1529	74.5466	757.6886	29.0107
v33	767.9072	41.1174	773.9480	10.5446	766.5300	57.6448
v34	826.4186	22.9266	825.3867	41.0766	819.4864	4.5012
v35	838.1347	0.1330	837.6937	0.5571	837.0654	0.1860
v36	871.4409	44.0775	869.1818	42.3174	868.9151	80.9304
v37	890.1753	15.7836	888.8573	4.3302	906.1565	15.0755
v38	908.4346	11.4895	906.5481	4.9802	909.2780	1.5019
v39	923.8784	6.9626	929.4229	12.9140	961.4110	67.0224
v40	951.7219	19.9872	954.8272	14.4856	971.3432	2.1173
v41	972.2219	0.1506	970.9494	0.2435	985.6414	49.3874
v42	993.0679	97.7847	991.9221	3.0556	992.6661	0.1837
v43	993.8880	7.9332	995.3263	70.0776	1013.9476	3.5050
v44	1014.8064	0.7601	1014.5597	3.8702	1021.8537	33.0929
v45	1032.0517	115.0931	1030.6760	312.7135	1031.2440	138.2757
v46	1050.7778	5.8093	1040.0758	106.8980	1052.5773	35.4196
v47	1055.6732	98.9763	1052.2092	64.5679	1071.2623	148.8960
v48	1096.4021	250.5428	1077.8321	101.2242	1076.3768	13.6018
v49	1104.6348	136.7593	1097.8252	112.6574	1094.5976	255.7428
v50	1110.3398	58.7363	1108.2693	2.8766	1109.3835	9.9849
v51	1122.6201	105.0159	1119.4921	44.3083	1120.3767	96.9651
v52	1142.4264	3.7286	1125.9048	65.7696	1136.7173	121.4885
v53	1146.7506	97.2084	1133.9233	73.1256	1142.3878	4.3655
v54	1152.2071	21.4914	1156.7025	16.6306	1153.3543	53.8010
v55	1188.3222	2.9896	1187.6574	2.9377	1188.1430	2.9192
v56	1206.8202	15.3423	1203.6357	15.3874	1205.2184	19.7124
v57	1221.9049	24.6833	1236.6666	21.3926	1219.9857	24.8713
v58	1239.6769	72.0858	1241.5299	17.7471	1243.8129	24.0271
v59	1251.9489	246.5442	1260.7440	141.6134	1249.4618	262.5732
v60	1267.8101	96.3807	1263.1508	208.2743	1257.0843	84.9797
v61	1284.9562	15.2570	1283.4024	66.5084	1271.1052	62.4193
v62	1313.3569	14.3908	1320.1374	4.7534	1281.5082	27.6390
v63	1332.7123	19.3868	1338.4948	9.8872	1316.8462	5.6310
v64	1346.7102	3.1311	1343.0910	3.5857	1344.2124	37.8160
v65	1365.8241	4.0469	1363.0626	4.2094	1347.1481	2.1738
v66	1368.5606	0.9982	1365.1670	7.9615	1358.4035	1.1924
v67	1374.4328	31.0937	1368.8994	8.9270	1365.7523	4.5698
v68	1387.5270	20.1058	1387.6587	22.2910	1373.7542	32.0959
v69	1391.5545	28.4582	1396.5063	78.6074	1394.1599	26.2141
v70	1405.3824	16.6217	1403.7256	9.2965	1400.6483	11.7675
v71	1409.9723	8.6801	1425.2259	21.1182	1414.8300	6.2627
v72	1431.8798	11.8087	1429.0159	39.0801	1432.1475	11.1635
v73	1441.6855	11.4830	1436.8968	24.8778	1441.3808	20.0104
v74	1445.2951	22.2655	1442.4289	45.7287	1445.5220	17.7771
v75	1471.6051	90.8820	1459.2263	20.2197	1462.7938	3.2704

v76	1498.3522	0.7760	1497.9406	0.4319	1498.3257	0.5774
v77	1516.1595	5.3970	1512.9342	5.3527	1535.8380	97.9140
v78	1535.9590	96.3548	1535.8854	101.3495	1537.8090	9.1762
v79	1639.3990	23.0557	1638.0331	21.7547	1639.0954	22.8375
v80	1651.8231	61.5193	1652.5183	67.9973	1652.1227	63.7680
v81	2981.1814	46.5644	2998.5422	39.5984	3021.8378	22.3069
v82	3008.0454	15.9706	3027.5914	22.7574	3037.7735	14.0996
v83	3019.1325	33.3948	3033.6737	18.2682	3039.2199	43.6570
v84	3033.2783	65.6595	3058.9395	47.6035	3051.8728	36.4193
v85	3096.3994	18.0292	3101.5333	18.2466	3094.6991	20.1492
v86	3104.7351	29.6386	3106.8024	20.2660	3102.1671	23.6570
v87	3119.4126	11.5827	3125.0362	18.7675	3121.7662	11.5843
v88	3184.8070	1.5801	3182.6946	1.5094	3184.1037	1.5679
v89	3192.5515	9.7158	3191.1176	15.0784	3191.8216	11.1328
v90	3203.6646	23.8671	3206.0617	28.3074	3203.8946	24.6554
v91	3212.1051	15.4286	3215.0762	7.5668	3211.8433	14.8690
v92	3232.8635	0.4843	3227.3820	3.0911	3233.3878	1.1042
v93	3699.4246	183.4854	3608.3484	267.9065	3708.1788	46.1237
v94	3706.4418	53.6530	3686.6946	55.9714	3717.0171	69.1948
v95	3710.5947	5.0084	3714.0393	50.0624	3718.5896	36.8226
v96	3717.9690	49.5640	3733.9895	36.1941	3781.6166	42.5777

Table 7. α -PhGal·D₂O

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	1.04	0.00
B	8.04	1.65
C	7.73	1.95
D	11.17	2.30
E	11.86	2.48
F	0.31	2.58



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.091507	-0.435145	0.753639
6	-0.965867	-1.531237	0.910360
6	-1.693188	-1.778539	-0.418493
6	-2.286817	-0.466717	-0.950177
6	-1.214383	0.637837	-0.974742
8	-0.548528	0.763872	0.307214
8	-0.350751	-2.707160	1.403783
8	-2.701440	-2.770552	-0.238666
8	-3.398748	-0.167283	-0.109348
6	-1.749936	2.014763	-1.379356
8	-2.879855	2.452450	-0.624497
1	-1.007498	-3.420275	1.322384
1	-3.486409	-2.309679	0.110740
1	-2.556955	2.817775	0.230562
1	0.549937	-0.181609	1.715119
1	-1.697467	-1.149389	1.637526
1	-0.984108	-2.192056	-1.141942
1	-2.632732	-0.621563	-1.985436
1	-0.457300	0.354219	-1.719494
1	-3.597195	0.788408	-0.209387
1	-2.078776	1.956248	-2.422595
1	-0.936641	2.749575	-1.321321
8	1.071175	-0.874954	-0.152385
6	4.951220	0.669135	-0.186525
6	3.919696	1.446889	0.341425
6	2.603613	0.970146	0.370075
6	2.332868	-0.310015	-0.124303
6	3.358767	-1.097914	-0.658384
6	4.662148	-0.604663	-0.690164
1	5.968577	1.049710	-0.208568
1	4.128978	2.441557	0.726911
1	1.805477	1.598548	0.749090
1	3.117984	-2.089948	-1.028457
1	5.456434	-1.222109	-1.101802
8	-1.518461	2.975184	1.737262
1	-1.956591	2.842165	2.591096
1	-1.080612	2.128724	1.508540

B			
6	0.260867	-0.931124	-0.668379
6	1.503849	-1.744352	-0.282656
6	2.333887	-1.012648	0.777245
6	2.671125	0.411426	0.320354
6	1.380821	1.131946	-0.076153
8	0.604608	0.380346	-1.037087
8	1.163701	-3.056740	0.157157
8	3.569525	-1.688910	1.005737
8	3.572315	0.395218	-0.780102
6	1.621013	2.485321	-0.733798
8	0.381364	3.155349	-1.003438
1	0.434563	-2.961501	0.796276
1	3.376226	-2.640066	1.070025
1	-0.153069	2.557087	-1.553683
1	-0.236446	-1.357958	-1.544440
1	2.113039	-1.874936	-1.180943
1	1.759392	-0.955159	1.713792
1	3.120311	0.956824	1.166279
1	0.776309	1.273633	0.828732
1	4.276393	-0.237655	-0.554951
1	2.193673	2.357798	-1.657830
1	2.179342	3.137575	-0.057032
8	-0.618309	-0.981616	0.455514
6	-4.699616	-0.336360	-0.186761
6	-4.106855	-1.530728	-0.608121
6	-2.740831	-1.746080	-0.407473
6	-1.973636	-0.753613	0.209165
6	-2.549724	0.443465	0.635711
6	-3.919599	0.642795	0.435518
1	-5.763099	-0.172594	-0.339436
1	-4.707207	-2.301133	-1.085295
1	-2.274103	-2.678502	-0.714967
1	-1.943325	1.207843	1.113539
1	-4.372987	1.573348	0.767079
8	-0.899980	3.312090	1.493944
1	-0.520198	3.433841	0.596364
1	-1.132414	4.195380	1.814781

C			
6	-0.037071	-0.425013	0.736439
6	-1.155681	-1.452807	0.951303
6	-1.945419	-1.680486	-0.341245
6	-2.445851	-0.354618	-0.921221
6	-1.281148	0.634602	-1.051584
8	-0.531624	0.752849	0.163123
8	-0.668980	-2.687665	1.467605
8	-3.094129	-2.492074	-0.097829
8	-3.460866	0.209788	-0.086424
6	-1.717308	2.059809	-1.412152
8	-2.351064	2.742485	-0.336586
1	0.138341	-2.910943	0.971078
1	-2.817917	-3.228454	0.474963
1	-3.052475	2.156626	0.004563
1	0.407880	-0.121452	1.688584
1	-1.830103	-1.051259	1.712613
1	-1.295330	-2.165205	-1.084825
1	-2.861057	-0.536050	-1.924706
1	-0.626708	0.264686	-1.855903
1	-4.070371	-0.510941	0.152384
1	-2.371734	2.019680	-2.296033
1	-0.833917	2.652037	-1.665575
8	0.947984	-1.067673	-0.069154
6	4.866767	0.368502	-0.299306
6	3.871775	1.195497	0.224793
6	2.543487	0.762284	0.315167
6	2.227258	-0.530146	-0.117512
6	3.213186	-1.368207	-0.650015
6	4.529112	-0.915723	-0.740700
1	5.892818	0.719364	-0.366974
1	4.117762	2.198503	0.563645
1	1.781268	1.433870	0.695901
1	2.937344	-2.365127	-0.982556
1	5.292164	-1.571499	-1.152303
8	-0.262450	3.297708	1.697701
1	-0.509432	4.203212	1.935986
1	-0.944144	3.007438	1.057858

D			
6	0.184334	-0.312343	-0.845816
6	1.441973	-1.196306	-0.797850
6	2.318981	-0.850656	0.411174
6	2.635927	0.651507	0.438311
6	1.335360	1.451708	0.337948
8	0.526544	1.044895	-0.790038
8	1.180942	-2.586873	-0.883706
8	3.564102	-1.544154	0.334968
8	3.503710	1.006427	-0.629668
6	1.543453	2.952568	0.168838
8	0.306459	3.657902	0.219574
1	0.722287	-2.892081	-0.069363
1	3.374319	-2.444388	0.017164
1	-0.243374	3.326729	-0.509282
1	-0.346337	-0.447101	-1.792562
1	2.005015	-0.948119	-1.703020
1	1.800931	-1.123421	1.342109
1	3.110643	0.894298	1.403487
1	0.759192	1.278726	1.257387
1	4.197537	0.324001	-0.658785
1	2.075542	3.146660	-0.769788
1	2.148469	3.333664	0.996933
8	-0.703359	-0.679900	0.232167
6	-4.723316	0.413903	-0.131481
6	-3.864540	1.157485	0.683572
6	-2.514985	0.809398	0.792292
6	-2.036185	-0.291781	0.081359
6	-2.884197	-1.046246	-0.733909
6	-4.230608	-0.686561	-0.839686
1	-5.771074	0.689741	-0.213811
1	-4.241636	2.014826	1.234827
1	-1.836138	1.383212	1.415385
1	-2.489040	-1.904027	-1.271989
1	-4.894109	-1.270766	-1.471986
8	-0.148718	-3.101505	1.558949
1	-0.623819	-2.268694	1.371360
1	-0.823038	-3.783639	1.695461

E			
6	0.420847	-0.821413	-0.899037
6	1.713746	-1.569282	-0.546337
6	2.378077	-0.959486	0.693160
6	2.581816	0.551029	0.517144
6	1.251096	1.198339	0.130777
8	0.652061	0.555898	-1.023624
8	1.499444	-2.967637	-0.377002
8	3.663261	-1.538441	0.911232
8	3.557221	0.820465	-0.482375
6	1.372548	2.670598	-0.243668
8	0.087057	3.243556	-0.516463
1	0.723927	-3.076786	0.201199
1	3.577750	-2.500425	0.795604
1	-0.279636	2.771559	-1.282053
1	0.027823	-1.152619	-1.865719
1	2.394313	-1.470521	-1.396081
1	1.736960	-1.127696	1.571187
1	2.901800	0.977969	1.481340
1	0.559228	1.106811	0.977452
1	4.314621	0.237890	-0.298354
1	2.036822	2.790297	-1.105834
1	1.782277	3.233355	0.599237
8	-0.509954	-1.143785	0.133280
6	-4.610579	-0.396643	-0.165423
6	-4.065435	-1.102331	0.913844
6	-2.692956	-1.334847	0.985267
6	-1.851749	-0.857887	-0.027625
6	-2.381524	-0.140497	-1.105736
6	-3.763567	0.077259	-1.168063
1	-5.680489	-0.217344	-0.220234
1	-4.710997	-1.475480	1.704554
1	-2.257050	-1.879052	1.817999
1	-1.737023	0.259042	-1.879766
1	-4.171622	0.632344	-2.008915
8	-1.452674	2.536425	1.834355
1	-1.069608	2.911281	1.015657
1	-2.234344	2.038491	1.551679

F			
6	-0.049252	-0.133904	0.860516
6	-1.436405	-0.790467	0.749386
6	-2.193579	-0.320039	-0.505575
6	-2.174068	1.216396	-0.598728
6	-0.754257	1.759237	-0.450824
8	-0.108530	1.256146	0.744787
8	-1.287299	-2.218334	0.801679
8	-3.566069	-0.680905	-0.474122
8	-3.007560	1.783406	0.404377
6	-0.687237	3.278955	-0.345610
8	0.655590	3.751009	-0.378096
1	-0.536359	-2.440743	0.221545
1	-3.672946	-1.658651	-0.496842
1	1.125315	3.347418	0.369195
1	0.395771	-0.340920	1.838988
1	-2.014949	-0.512786	1.633444
1	-1.702445	-0.734392	-1.399028
1	-2.543520	1.499774	-1.597691
1	-0.165133	1.438443	-1.320548
1	-3.834008	1.268354	0.392723
1	-1.188652	3.724943	-1.209627
1	-1.205125	3.606166	0.563719
8	0.744697	-0.749114	-0.158919
6	4.923485	-0.745687	-0.087336
6	4.203024	-1.553434	-0.974446
6	2.809272	-1.532867	-0.974887
6	2.126084	-0.696313	-0.084548
6	2.832600	0.126538	0.798210
6	4.231972	0.087927	0.792321
1	6.009600	-0.763124	-0.087560
1	4.726904	-2.205510	-1.668518
1	2.237954	-2.155704	-1.657481
1	2.313391	0.802946	1.467288
1	4.778907	0.728510	1.479405
8	-3.529690	-3.466029	-0.223820
1	-2.739887	-3.289548	0.331559
1	-4.183757	-3.902663	0.341467

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	27.5441	1.1343	30.8822	0.3385	14.1605	1.5503
v2	29.7832	1.6790	39.3723	1.2543	24.6998	0.9190
v3	43.3399	0.0294	52.3965	0.5288	32.3936	0.3013
v4	56.5323	2.4041	54.7313	2.3738	54.9800	0.1586
v5	83.1598	4.8225	77.5733	3.7677	62.7386	0.8048
v6	122.0660	11.1011	92.6267	1.6022	109.0718	1.3118
v7	136.9861	5.7367	106.2779	11.1507	116.3766	7.5594
v8	140.6947	5.5252	120.0828	37.6659	120.2161	5.3003
v9	158.0915	7.2231	126.2189	0.0904	139.1401	62.3826
v10	190.9537	0.8732	134.3158	26.9408	141.0911	0.6004
v11	208.2962	34.1721	162.8057	1.3846	171.6589	11.7731
v12	217.1731	1.8458	186.1805	2.6561	191.6328	63.3544
v13	240.9838	33.7668	221.9746	8.4717	193.3044	0.7874
v14	258.9153	5.1925	236.8943	3.9092	215.4218	1.3547
v15	273.2169	9.1278	253.8300	3.0666	251.3130	2.4171
v16	280.9816	9.1651	265.8651	21.5884	263.4993	6.1959
v17	299.2486	6.9736	287.0636	87.3044	268.6537	3.5387
v18	307.7205	71.6061	308.6639	0.3413	289.0282	2.2601
v19	337.0846	1.4448	334.5925	18.6481	322.0167	10.1992
v20	366.1185	5.9086	370.6919	3.9089	355.8898	6.3681
v21	378.6186	20.0196	385.4518	8.7337	379.1873	12.5745
v22	387.7358	30.1800	405.7876	42.4053	403.8480	34.9823
v23	424.2680	0.0683	426.8773	1.6704	423.9317	23.5982
v24	432.4752	9.2504	434.0103	48.2912	426.2476	5.3693
v25	463.6639	31.7995	443.6373	50.1620	446.5326	79.4604
v26	499.5901	5.6860	457.4424	117.4210	461.5964	88.2698
v27	514.3986	17.6563	469.9507	18.8349	489.2684	175.0945
v28	523.7887	174.0628	481.8534	32.0362	500.8825	16.1231
v29	538.4869	1.3546	513.5344	151.9826	521.5218	6.2952
v30	569.9122	1.3143	549.4710	16.7266	537.7357	12.5257
v31	604.3857	164.1475	554.8450	11.5124	567.4653	27.2411
v32	626.9687	1.0953	576.7555	113.3238	612.8454	126.4588
v33	656.5290	16.2991	627.8785	1.3803	627.0564	11.8618
v34	700.5872	12.2562	657.1574	23.2443	655.2161	4.2564
v35	707.0150	24.4468	685.7048	58.2371	703.1329	18.5662
v36	746.5547	16.0878	706.3516	21.0335	708.2379	16.3642
v37	765.1781	52.0791	715.9446	14.0197	755.5459	6.3451
v38	772.0224	29.0011	762.9350	30.0855	763.7370	74.4277
v39	830.9560	69.9389	790.5749	44.8594	768.5032	44.2533
v40	839.6412	0.8894	813.0336	11.6564	825.2456	19.7543
v41	852.7580	120.8417	856.4978	1.1102	845.3536	0.0239
v42	868.7141	37.4994	864.0714	54.5642	872.3243	56.1159
v43	885.5339	11.0193	893.4345	23.0543	895.3944	10.7334
v44	909.4714	3.6030	923.2556	34.4658	916.2205	11.0084
v45	926.4672	15.8250	940.8601	4.6235	929.5017	2.0697
v46	956.4276	16.6346	979.4588	59.1091	951.3545	22.1968
v47	972.7168	0.2774	986.6239	6.3758	976.9642	0.0080
v48	993.2630	0.2659	1007.0470	16.6941	995.9615	58.9883
v49	999.1786	30.6645	1013.3845	7.2157	997.5803	17.6696
v50	1013.9972	138.6094	1017.7405	4.0859	1013.8418	1.8379
v51	1019.3628	305.8617	1040.9621	192.9466	1035.8697	95.3570
v52	1045.1133	5.3132	1048.5774	20.0770	1049.6963	22.0667
v53	1051.5145	33.6710	1055.4229	95.3816	1055.4286	138.7780
v54	1091.3033	145.1926	1089.4257	186.9644	1098.6107	188.6175
v55	1103.4153	68.2430	1095.7046	74.4645	1101.4282	208.0969
v56	1108.3410	12.5039	1107.0582	5.0711	1111.8786	40.5883
v57	1118.0097	58.0527	1124.5629	182.3830	1120.5352	31.0740
v58	1127.8903	46.7089	1135.5332	28.1699	1131.7277	78.5838
v59	1135.1570	57.9514	1140.6576	11.0139	1143.9155	39.3046
v60	1166.7888	29.0003	1147.9595	68.5219	1155.2450	69.6500
v61	1187.8819	3.2505	1188.2645	0.7437	1187.4620	3.0709
v62	1202.3021	17.2224	1201.0291	16.9133	1211.5747	17.6201
v63	1225.4016	26.8299	1219.8583	35.9848	1220.5510	27.8785
v64	1239.7525	11.5709	1228.8011	29.1844	1231.0074	63.9722
v65	1258.2181	298.6717	1232.6078	43.9844	1238.8028	88.8602
v66	1264.9111	20.9112	1236.9797	191.3375	1248.0661	199.8403
v67	1275.2646	36.2421	1259.8450	17.1296	1265.8100	103.2265
v68	1289.7404	75.9910	1267.2348	69.8941	1280.0696	13.8453
v69	1322.0144	4.4160	1314.3554	33.5723	1312.3417	13.7313
v70	1341.7290	2.6535	1327.9313	7.4073	1330.9101	21.7746
v71	1345.7682	2.6955	1336.9730	2.0654	1346.9845	4.5022
v72	1363.6030	6.3749	1362.2846	3.1822	1364.2974	2.4969
v73	1365.7775	2.4945	1364.9069	31.1960	1370.0058	2.3503
v74	1372.9087	28.9549	1367.2654	16.8231	1378.7059	17.2531
v75	1387.5718	46.6484	1394.5033	18.6466	1383.4500	8.9719

v76	1404.0520	24.2396	1395.7779	9.2761	1397.1330	36.4028
v77	1420.3553	8.7816	1404.0757	28.4851	1405.4613	22.9628
v78	1424.1965	12.3047	1405.0347	12.5200	1412.3671	7.9521
v79	1440.4702	18.9662	1432.2240	8.6653	1432.8017	10.5849
v80	1444.1490	71.2150	1434.4560	22.0536	1440.5546	14.7767
v81	1468.7710	7.9277	1444.4461	21.8772	1447.4506	18.9306
v82	1494.0565	69.3190	1455.5669	16.8795	1469.2487	84.6207
v83	1497.8987	0.5051	1492.8250	2.2635	1498.3856	1.4085
v84	1509.0453	9.5913	1516.3948	2.5087	1518.5360	6.8819
v85	1535.6378	98.9627	1535.5393	66.4708	1536.7524	88.3767
v86	1638.9559	21.4558	1640.7737	8.2783	1639.3118	25.9096
v87	1652.1279	61.9376	1645.6791	37.2372	1651.2774	51.1301
v88	2599.5325	159.7311	2566.2614	186.7234	2616.7182	145.0295
v89	2791.0899	103.2873	2792.1003	67.3710	2790.7114	69.4454
v90	2995.4696	40.8669	2999.1648	36.1722	3009.3211	11.5992
v91	3025.7396	24.5544	3026.9893	29.5645	3017.2495	2.5656
v92	3040.2183	6.1666	3068.4545	8.6939	3025.2875	34.0767
v93	3055.4105	51.0570	3086.9425	22.4843	3034.0410	99.4069
v94	3090.7893	19.7811	3100.2074	16.3955	3106.2148	9.4305
v95	3106.6260	21.5642	3119.6535	12.7017	3116.9638	13.2053
v96	3107.0313	24.9594	3141.4640	15.8445	3121.5063	21.2926
v97	3184.6125	0.7731	3182.0395	1.1155	3183.7746	1.3376
v98	3193.0107	14.3125	3190.8286	10.9449	3193.2661	10.9087
v99	3207.4012	27.1100	3199.0709	31.2204	3202.8937	26.6708
v100	3216.3149	6.8141	3207.9304	8.2293	3211.0967	14.5197
v101	3229.7778	2.5471	3213.1711	17.2921	3225.9311	4.0861
v102	3492.5326	521.5508	3695.4941	47.7382	3675.7165	152.6534
v103	3549.2860	274.7116	3709.9729	64.0780	3704.7182	53.8603
v104	3685.8154	57.8647	3717.8366	46.8312	3708.9414	56.8946
v105	3711.8677	52.4359	3724.9186	43.6607	3715.4463	47.4315

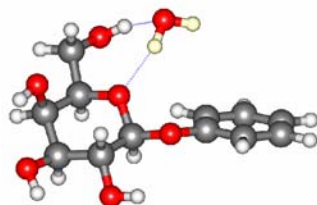
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	27.3991	0.0236	24.7449	0.5657	30.5566	0.2253
v2	33.2603	0.2244	32.2290	8.7036	37.9259	0.8859
v3	39.0874	0.7557	43.7126	0.8996	49.6483	0.1855
v4	61.7595	3.6599	54.7874	3.8579	55.0449	0.0719
v5	80.5614	2.1595	59.6353	10.0484	98.0358	5.3228
v6	100.6825	2.0154	91.5747	19.9104	107.3914	3.6011
v7	120.5047	0.9025	105.0931	45.0853	121.9188	7.0377
v8	130.6075	2.2586	116.0058	10.7623	138.1358	1.0021
v9	137.8552	11.5513	129.1938	3.6162	146.7667	14.3319
v10	145.9453	13.3872	138.2529	0.3404	156.4678	0.0967
v11	179.3495	2.8907	160.3620	1.3304	172.5306	1.3336
v12	189.8337	53.1928	190.5444	2.6553	206.6644	64.9400
v13	231.0573	37.5287	201.6617	4.3876	235.5039	61.8690
v14	235.9940	3.3477	238.1037	10.9986	246.6859	9.8075
v15	258.0392	23.4450	247.1320	4.7890	269.6006	17.6706
v16	267.5839	10.1608	261.4654	2.8653	274.4277	51.1375
v17	274.0160	37.4663	268.6233	8.2728	291.0305	2.9446
v18	308.9697	4.3009	286.5733	2.0544	332.4836	19.7357
v19	337.6971	26.8297	337.5502	18.3922	350.3074	15.8505
v20	364.2720	4.8930	361.6853	8.1291	360.1775	0.6357
v21	386.0648	54.9742	373.9009	12.5709	376.9783	113.2531
v22	394.3444	20.9259	395.9202	37.6413	400.2104	42.7993
v23	403.7189	128.0790	420.0390	8.8309	417.3018	14.4660
v24	425.9399	0.5959	422.2115	2.1937	423.7695	4.2607
v25	432.2464	74.2673	435.8675	111.8490	456.3090	165.3983
v26	443.8291	18.2264	447.4488	74.4599	474.6549	12.2195
v27	467.0719	111.9963	466.1415	149.7453	497.5011	40.9998
v28	481.4843	28.4188	490.4115	174.4264	518.6572	5.5490
v29	486.1918	20.5155	497.9120	104.2390	537.2512	14.8796
v30	547.9122	1.9612	519.0636	7.1056	550.5267	42.7610
v31	558.3939	3.2364	535.9424	16.8594	551.3257	52.3169
v32	628.1472	0.9660	552.8646	13.6750	627.5439	0.4395
v33	664.0909	13.8346	627.4700	0.5451	673.8709	13.7333
v34	687.1108	55.1323	674.3736	13.6330	697.3316	53.5227
v35	704.2285	19.7843	690.8139	64.7993	702.1997	20.7693
v36	713.4970	25.0092	694.8640	15.3893	706.7742	4.9701
v37	749.8598	12.9550	708.9577	3.5769	756.8591	113.5033
v38	772.2597	190.0646	763.9677	75.7631	765.3630	68.7040
v39	793.4744	51.0944	775.6652	24.8576	775.6198	26.4971
v40	811.9903	8.7514	809.5648	8.5731	814.9479	13.7817
v41	848.6869	0.4695	837.5142	1.4751	837.9454	0.7982
v42	862.8475	53.0471	860.4654	76.5958	864.7847	71.4789
v43	883.8007	59.5012	895.8619	8.8972	893.8996	15.0836
v44	911.9135	51.7600	904.5021	8.2702	907.0593	10.1924
v45	936.5294	9.9551	935.0918	26.1582	930.2801	30.3719
v46	971.4422	92.6828	972.9700	0.2009	971.9890	0.0055
v47	979.6604	0.2732	983.4950	42.8772	979.3218	56.7109
v48	1001.5750	0.4323	993.4691	0.1002	994.2342	0.1802
v49	1008.6759	28.8868	1009.7404	16.1343	1013.7737	6.9967
v50	1018.5274	1.4576	1014.3346	0.8331	1014.9756	1.4523
v51	1040.3037	173.9114	1043.8968	165.9757	1045.3088	128.6779
v52	1047.8996	6.9535	1053.7974	80.3850	1053.4399	63.7984
v53	1070.3178	85.4251	1057.0617	64.5659	1068.3887	236.1180
v54	1094.0666	28.6209	1088.8838	88.7542	1079.8507	49.1984
v55	1102.3904	32.4264	1096.6668	178.4814	1097.7572	46.9714
v56	1107.7255	180.3218	1110.1583	18.1324	1111.4505	17.9040
v57	1128.1984	190.6374	1125.1607	189.9645	1130.6130	261.0647
v58	1139.0199	4.0947	1133.6503	15.6389	1131.9990	17.5007
v59	1143.3155	8.8879	1140.8109	8.7818	1148.7819	53.3264
v60	1154.5663	51.7730	1149.2758	53.3212	1158.8810	26.3887
v61	1189.7494	0.0911	1188.7655	3.0223	1188.7274	3.2169
v62	1194.2690	12.6409	1205.9690	23.5460	1206.7325	22.3479
v63	1211.9551	1.2413	1221.7439	32.3494	1218.4207	54.3581
v64	1227.6359	62.6807	1227.0033	20.8119	1231.1867	40.9514
v65	1234.8964	11.1526	1247.0466	44.7055	1237.1099	51.3494
v66	1239.8834	173.0870	1254.1788	284.5992	1252.6827	223.8872
v67	1263.9084	26.3975	1263.6866	11.5782	1268.2326	88.5414
v68	1293.0165	27.8874	1269.5175	69.6719	1286.3750	2.8025
v69	1325.9075	15.7142	1314.6092	17.2174	1313.0900	25.7131
v70	1334.3667	2.1249	1329.8586	20.2004	1317.7830	11.3985
v71	1355.4727	11.1868	1348.3702	5.5318	1347.5105	4.6204
v72	1359.2155	0.8431	1365.6007	2.8239	1365.4798	3.5038
v73	1368.4638	26.4037	1372.4299	8.8548	1369.2987	7.3389
v74	1369.8610	8.4606	1377.4688	37.0465	1375.7595	39.1869
v75	1392.9681	25.6015	1390.3295	20.0065	1390.2620	51.0886

v76	1394.5621	17.0795	1397.6457	17.1220	1394.0032	23.8343
v77	1400.1551	16.9537	1404.9693	28.8371	1402.7809	1.2322
v78	1406.7015	17.4314	1415.4721	9.5868	1426.5613	1.5242
v79	1432.8406	20.9627	1432.8854	11.8698	1436.1508	15.8268
v80	1443.4938	10.3312	1433.9399	15.3059	1438.4141	23.8200
v81	1450.2982	16.0916	1447.4047	22.8466	1453.3233	23.4847
v82	1483.0300	46.5248	1454.5238	15.0407	1466.3886	51.4551
v83	1492.9775	1.3253	1498.1657	0.7154	1499.0996	0.6037
v84	1515.5063	2.0022	1515.5629	2.4544	1515.3211	2.4354
v85	1534.0861	68.9412	1536.1872	98.0259	1536.4094	98.0114
v86	1641.1331	7.1250	1638.7240	23.7594	1640.6264	25.6414
v87	1645.8884	37.9712	1651.9204	63.0202	1652.5029	62.4031
v88	2637.2756	93.3454	2610.3943	109.9300	2579.5967	179.3453
v89	2799.1509	97.2087	2787.8452	55.3692	2792.0470	102.1915
v90	2991.9812	40.0058	3002.3661	32.5756	2998.8555	33.4546
v91	3032.1790	13.7105	3027.7232	33.7061	3022.9758	29.3156
v92	3046.5616	29.7571	3070.5294	5.1778	3051.8114	19.3307
v93	3068.9751	31.9660	3084.5111	19.7429	3068.3574	32.3923
v94	3097.9479	13.1156	3092.3221	21.9809	3092.2828	20.7290
v95	3108.5916	21.8183	3120.4851	11.0074	3125.2273	21.2731
v96	3124.9370	22.7151	3141.0115	13.5250	3128.6708	10.4244
v97	3185.6141	1.4191	3187.1006	1.6826	3185.9624	2.0122
v98	3193.9760	5.7792	3194.6086	9.9155	3193.2330	9.0967
v99	3202.3906	18.0486	3207.6908	20.4954	3204.7413	21.6314
v100	3210.9406	17.7840	3215.0921	11.4167	3213.2463	16.2276
v101	3220.4734	2.4231	3234.2859	3.7589	3232.8862	3.2293
v102	3519.5615	420.5635	3708.8251	44.5365	3500.7984	708.8992
v103	3701.0793	69.8837	3710.8231	64.1540	3692.3739	78.8508
v104	3707.9737	44.5157	3718.3290	47.5088	3700.2327	62.4626
v105	3740.4070	27.4114	3743.8230	30.6771	3750.1832	24.9637

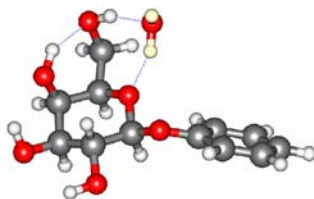
Table 8. β -PhGal $\cdot$ D₂O

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

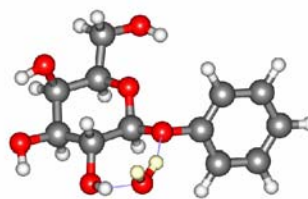
Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	6.59	0.00
B	0.00	0.38
C	8.24	0.67
D	8.57	1.58
E	9.02	3.65
F	8.98	3.79



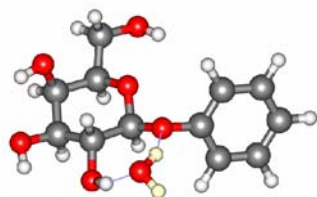
A



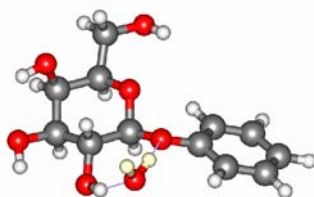
B



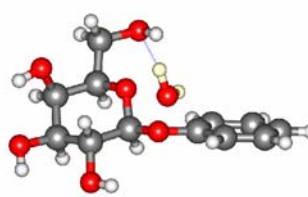
C



D



E



F

(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	-0.210012	-0.725057	-0.204147
6	-1.366344	-1.657194	0.162740
6	-2.627722	-1.210481	-0.574597
6	-2.933229	0.270184	-0.308048
6	-1.684642	1.122061	-0.571719
8	-0.545969	0.605200	0.152869
8	-1.119877	-3.004802	-0.231167
8	-3.765214	-1.959745	-0.155923
8	-3.364817	0.467515	1.030474
6	-1.858851	2.593598	-0.190009
8	-0.774157	3.391721	-0.627856
1	-0.360353	-3.338144	0.273242
1	-3.524736	-2.901428	-0.174347
1	-0.075028	3.347562	0.057119
1	-1.525606	-1.587802	1.246328
1	-2.466479	-1.352531	-1.655103
1	-3.719220	0.592380	-1.010171
1	-1.455068	1.073394	-1.648674
1	-4.022615	-0.223732	1.220215
1	-2.761415	2.966192	-0.687973
1	-2.013186	2.675456	0.892295
8	0.907293	-1.128268	0.540835
1	0.014985	-0.782486	-1.282109
6	4.809903	-0.053400	-0.499100
6	3.743310	0.635603	-1.078187
6	2.418625	0.313901	-0.756277
6	2.173440	-0.723646	0.149759
6	3.234803	-1.419328	0.739321
6	4.547601	-1.080477	0.415044
1	5.833534	0.207115	-0.752711
1	3.931871	1.440375	-1.784117
1	1.603502	0.883294	-1.188952
1	3.015341	-2.215752	1.444410
1	5.368091	-1.624494	0.875583
8	0.937963	2.643202	1.513862
1	0.578625	1.758778	1.304951
1	1.894694	2.568657	1.376583

B			
6	0.053669	-0.675448	-0.215399
6	-0.983910	-1.681236	0.280267
6	-2.273868	-1.574487	-0.549633
6	-2.804565	-0.139656	-0.577379
6	-1.680762	0.820208	-1.010739
8	-0.498436	0.647224	-0.211434
8	-0.428643	-2.981923	0.161268
8	-3.245077	-2.487099	-0.046149
8	-3.321180	0.121370	0.722493
6	-2.077873	2.300307	-0.953276
8	-2.583544	2.709022	0.314793
1	-1.156695	-3.610649	0.306055
1	-3.681282	-2.043578	0.704558
1	-1.819362	2.853977	0.921201
1	-1.205160	-1.443424	1.329932
1	-2.056917	-1.906756	-1.572581
1	-3.612786	-0.069646	-1.324354
1	-1.432438	0.587372	-2.061716
1	-3.330346	1.094487	0.850809
1	-1.217000	2.916207	-1.244424
1	-2.879596	2.469425	-1.680456
8	1.133815	-0.670772	0.667816
1	0.388433	-0.931274	-1.232772
6	5.005785	0.334352	-0.534155
6	3.922531	0.833644	-1.259062
6	2.608865	0.522078	-0.890336
6	2.390593	-0.312088	0.210194
6	3.467544	-0.817107	0.945708
6	4.770422	-0.488707	0.573221
1	6.022057	0.585703	-0.824534
1	4.091647	1.483222	-2.114169
1	1.773893	0.947880	-1.436115
1	3.265088	-1.467068	1.791578
1	5.605043	-0.885536	1.145458
8	-0.189385	2.699271	1.694864
1	-0.002377	1.847587	1.250763
1	-0.083182	2.544160	2.645086

C			
6	-0.179756	-0.366506	-0.264186
6	-1.391059	-1.285654	-0.059698
6	-2.602061	-0.668204	-0.765837
6	-2.861050	0.770760	-0.308241
6	-1.564406	1.580442	-0.424171
8	-0.468468	0.924485	0.237611
8	-1.224748	-2.577825	-0.620162
8	-3.778350	-1.425328	-0.499143
8	-3.332836	0.805030	1.032033
6	-1.646517	2.974583	0.188545
8	-0.461443	3.722251	-0.061247
1	-0.675387	-3.120141	-0.012769
1	-3.540394	-2.362284	-0.613258
1	0.284090	3.206631	0.287617
1	-1.590121	-1.341516	1.019138
1	-2.401964	-0.665263	-1.849446
1	-3.608427	1.222919	-0.980630
1	-1.319545	1.681403	-1.494838
1	-4.005705	0.106149	1.108046
1	-2.466285	3.532094	-0.274074
1	-1.846486	2.887637	1.263148
8	0.919292	-0.871809	0.470764
1	0.092083	-0.307698	-1.331120
6	4.710477	0.667003	-0.388831
6	4.146624	-0.304533	-1.221335
6	2.873250	-0.812939	-0.949157
6	2.172376	-0.332743	0.157946
6	2.722423	0.633824	0.999698
6	3.998604	1.131483	0.721622
1	5.701848	1.057340	-0.602145
1	4.699783	-0.675416	-2.080173
1	2.428570	-1.581090	-1.575863
1	2.150708	0.980073	1.855081
1	4.434774	1.884595	1.372678
8	0.599694	-3.572704	1.238822
1	0.425449	-3.807569	2.162180
1	0.938453	-2.655770	1.238885

D			
6	-0.183869	-0.364227	-0.279944
6	-1.396795	-1.279104	-0.069791
6	-2.610335	-0.652999	-0.763118
6	-2.857571	0.785358	-0.295739
6	-1.557963	1.589971	-0.417254
8	-0.458810	0.925235	0.230740
8	-1.233566	-2.569184	-0.639579
8	-3.788507	-1.404572	-0.490204
8	-3.318357	0.815219	1.047807
6	-1.629728	2.980075	0.205992
8	-0.442621	3.724144	-0.045409
1	-0.707985	-3.119822	-0.018790
1	-3.552846	-2.343543	-0.592090
1	0.301110	3.207786	0.306080
1	-1.586331	-1.343977	1.009751
1	-2.419615	-0.645417	-1.848551
1	-3.607615	1.245055	-0.960231
1	-1.321351	1.697289	-1.489232
1	-3.985172	0.111105	1.129906
1	-2.449594	3.544561	-0.247901
1	-1.823778	2.886246	1.281010
8	0.917490	-0.881902	0.443109
1	0.077906	-0.300758	-1.349260
6	4.719967	0.650399	-0.375068
6	4.112880	-0.224653	-1.280961
6	2.834951	-0.729968	-1.024457
6	2.170956	-0.342384	0.141017
6	2.764491	0.528415	1.054730
6	4.045559	1.021900	0.792351
1	5.714627	1.038488	-0.576705
1	4.635368	-0.521995	-2.186438
1	2.357342	-1.421809	-1.713056
1	2.220049	0.806017	1.951954
1	4.514410	1.700474	1.500139
8	0.462679	-3.539262	1.350845
1	0.895765	-2.667554	1.260023
1	1.155994	-4.206285	1.238371

E			
6	-0.146142	-0.254917	-0.278172
6	-1.238074	-1.331874	-0.205824
6	-2.490991	-0.797598	-0.905101
6	-2.948491	0.535572	-0.302628
6	-1.763992	1.509078	-0.248585
8	-0.609176	0.916951	0.372003
8	-0.893222	-2.540743	-0.860351
8	-3.569037	-1.719242	-0.779632
8	-3.476518	0.348059	1.003637
6	-2.056241	2.784312	0.537686
8	-0.958903	3.690002	0.490685
1	-0.334096	-3.070169	-0.252729
1	-3.207295	-2.601892	-0.974199
1	-0.212237	3.261879	0.939829
1	-1.465251	-1.506249	0.854319
1	-2.255162	-0.646761	-1.970898
1	-3.719170	0.971678	-0.959000
1	-1.502278	1.785045	-1.284074
1	-4.054752	-0.433570	0.959106
1	-2.905652	3.304701	0.085494
1	-2.315994	2.524883	1.570307
8	1.002347	-0.709340	0.400589
1	0.118229	-0.034891	-1.325589
6	4.791516	0.851893	-0.440142
6	3.663174	1.636143	-0.685985
6	2.379108	1.150284	-0.415933
6	2.235367	-0.143347	0.093228
6	3.356769	-0.941858	0.338297
6	4.630972	-0.438128	0.076212
1	5.784821	1.239745	-0.647681
1	3.773246	2.642263	-1.082273
1	1.511323	1.778251	-0.581130
1	3.224533	-1.952063	0.714846
1	5.499496	-1.063301	0.266146
8	0.772363	-3.411506	1.235592
1	0.459534	-3.691162	2.108855
1	0.980027	-2.459200	1.300167

F			
6	0.183608	-0.702899	0.174813
6	1.354610	-1.687614	0.121657
6	2.600937	-1.028213	0.710633
6	2.907062	0.309321	0.020038
6	1.637253	1.169574	-0.013088
8	0.521870	0.455114	-0.569209
8	1.114246	-2.861646	0.893752
8	3.750613	-1.856843	0.551522
8	3.384533	0.105023	-1.302101
6	1.778627	2.432078	-0.858769
8	0.562053	3.191950	-0.854123
1	0.336427	-3.312364	0.526524
1	3.508365	-2.755369	0.832869
1	-0.116634	2.639873	-1.279404
1	1.530963	-1.941464	-0.931629
1	2.422113	-0.843002	1.781361
1	3.667313	0.840758	0.615691
1	1.390171	1.455864	1.021319
1	4.024186	-0.627195	-1.259015
1	2.058275	2.168603	-1.883473
1	2.549264	3.083389	-0.437648
8	-0.911029	-1.329389	-0.428764
1	-0.054411	-0.429400	1.215636
6	-4.847511	0.000626	0.021404
6	-4.540673	-1.182320	-0.660738
6	-3.215873	-1.594626	-0.794851
6	-2.188082	-0.820029	-0.245228
6	-2.474655	0.370172	0.430231
6	-3.811823	0.765303	0.560152
1	-5.880147	0.321822	0.126488
1	-5.334478	-1.788596	-1.089742
1	-2.960637	-2.509795	-1.321437
1	-1.697061	1.001802	0.846062
1	-4.031463	1.690001	1.087627
8	-0.519683	3.009257	1.742279
1	-0.172178	3.291101	0.868199
1	-0.761763	3.818010	2.216195

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	30.4482	0.4657	27.4777	0.1344	21.7678	0.1780
v2	41.2169	1.1843	35.4558	1.3522	29.9576	0.1605
v3	52.8883	0.4855	42.1215	0.0531	39.3884	1.6863
v4	59.2672	0.7744	55.9292	2.8814	52.6546	1.0201
v5	89.7617	3.3123	71.1413	3.1602	81.9822	1.2512
v6	100.3059	9.8039	106.4490	4.5240	103.5513	6.7073
v7	119.6851	2.0862	117.9004	5.2295	112.5381	3.5565
v8	140.2704	4.6266	138.9394	4.2603	131.6582	6.4325
v9	150.6956	4.3265	178.3754	11.6139	144.7211	4.5078
v10	182.1925	24.9932	189.2634	44.1727	158.4727	6.3302
v11	197.9932	2.4603	204.2019	1.2800	177.5364	34.6569
v12	209.3709	7.1552	237.0999	22.1375	183.7667	45.5144
v13	215.9135	11.1491	240.7031	1.5608	211.5086	1.5590
v14	239.4602	0.4915	248.2848	3.5268	221.9253	34.2526
v15	257.1445	9.3994	267.7628	9.8004	233.5460	12.3160
v16	264.6450	5.0107	282.9272	9.3257	254.3701	5.6033
v17	274.2224	32.3968	300.7466	21.3866	289.1591	18.7113
v18	288.2842	17.0230	305.2756	31.3604	304.1397	0.5786
v19	316.3843	12.5640	311.6172	6.9754	340.9678	8.2862
v20	351.8144	12.0657	342.4136	0.6477	379.5096	21.1961
v21	370.3913	100.4630	393.6099	16.4304	386.8174	28.1765
v22	391.0193	68.8031	402.8308	38.1435	407.9310	57.8422
v23	399.9719	33.5355	419.6831	50.4063	424.7262	0.2472
v24	404.3759	71.4508	424.1061	1.7126	427.2788	72.9761
v25	422.8854	44.0949	430.1915	12.5536	436.5926	164.3420
v26	426.5743	31.9399	487.8576	7.1062	448.4218	24.2985
v27	439.0572	100.3624	505.2621	14.1588	462.7631	94.5826
v28	474.0562	9.2736	517.5577	71.1032	472.7312	18.3132
v29	510.7968	20.1318	525.8016	102.4104	482.5142	17.3511
v30	519.9307	9.5748	583.4603	5.9040	523.2955	8.9871
v31	579.8887	2.3972	592.0765	36.7088	576.6105	5.4903
v32	605.6109	3.0352	611.3512	87.4926	605.5355	0.5495
v33	627.6204	1.4576	631.9222	2.8822	628.9168	5.5943
v34	634.8821	4.0758	647.0244	31.9254	631.0774	3.9512
v35	692.5208	51.8217	702.4776	24.3889	697.1514	40.5678
v36	697.6137	117.0402	746.0551	29.7492	707.5120	35.0515
v37	704.9890	77.6243	767.7147	59.2076	773.2179	95.5681
v38	764.5611	66.9556	806.3764	24.8367	785.6466	90.0064
v39	782.5176	47.7898	826.6398	7.9464	789.4328	15.2417
v40	832.0329	18.7948	837.8584	0.3804	838.0891	21.6767
v41	842.6254	0.3500	863.8930	109.8147	847.4005	0.1233
v42	883.9402	20.2727	874.4020	47.6194	878.6527	15.5296
v43	894.0680	24.4460	897.7716	23.2327	898.2754	18.9766
v44	910.1208	4.3895	908.4209	3.5680	930.3923	6.6378
v45	955.0191	22.0099	952.2980	36.2288	958.2253	22.7084
v46	975.9590	0.1207	966.5324	23.4803	978.6210	0.1567
v47	995.3425	0.0724	971.8837	0.1815	1000.0351	0.7923
v48	1014.1734	1.7665	993.5820	0.0926	1017.3918	17.8555
v49	1037.6161	7.7992	1015.1333	2.0639	1035.1243	14.0304
v50	1043.2312	4.3021	1032.9817	291.5238	1041.8194	102.5484
v51	1054.7133	13.9114	1040.8712	87.1051	1048.3167	75.3022
v52	1065.1843	275.3579	1052.9917	48.4504	1065.8192	156.4415
v53	1091.6756	27.4429	1072.2011	61.3054	1082.4702	127.8382
v54	1093.5850	99.2219	1097.4085	55.9584	1095.9563	132.4676
v55	1100.3976	279.4060	1105.7338	79.4668	1100.4543	25.9513
v56	1109.6755	5.2664	1107.2991	90.4541	1103.1526	149.5004
v57	1114.5504	50.7644	1118.9790	102.0026	1110.1450	7.2164
v58	1140.8296	80.6912	1127.3398	20.0273	1136.4704	62.3790
v59	1146.0397	10.9796	1150.0067	7.3557	1144.5090	42.4515
v60	1155.2544	12.1721	1169.2375	52.9148	1153.4329	2.6361
v61	1188.6721	2.8753	1188.0950	2.5448	1189.4334	1.1302
v62	1207.2916	15.8824	1202.7623	16.4735	1191.9942	19.7569
v63	1216.3135	94.8943	1225.3039	32.8654	1217.0442	59.6572
v64	1235.5510	36.3964	1243.2200	43.3154	1226.3882	102.7810
v65	1244.1004	5.4349	1262.5981	291.1207	1231.3488	85.0999
v66	1252.5007	278.7055	1268.4415	33.7107	1241.3523	79.5365
v67	1262.6813	107.0290	1272.4202	48.3447	1261.6574	25.9114
v68	1278.5770	28.0401	1290.6534	41.2656	1275.2743	3.4272
v69	1306.5816	29.0999	1314.5989	16.0018	1306.8776	24.2742
v70	1315.1258	9.8618	1334.8986	3.4008	1320.3495	23.7302
v71	1346.2510	5.1469	1344.2180	1.9193	1335.0419	0.3796
v72	1359.0854	24.9864	1347.2267	10.7506	1357.4251	2.2526
v73	1368.2306	3.2085	1365.1468	0.9238	1362.4411	10.8541
v74	1373.6214	20.3381	1373.2030	9.8321	1371.5064	18.6721
v75	1383.2073	2.8415	1379.4659	78.7683	1390.7725	5.2382

v76	1409.6853	35.2524	1403.6793	12.4039	1397.6186	10.4745
v77	1417.6855	20.3522	1410.3417	14.6696	1413.1853	18.1577
v78	1426.2390	1.6280	1419.0429	13.3506	1420.5144	108.3643
v79	1431.2406	28.1412	1441.3185	78.6285	1426.9003	6.6553
v80	1442.1615	3.6685	1457.4276	33.5930	1437.6939	4.1081
v81	1447.6749	32.0258	1470.0485	7.6680	1448.5610	15.0889
v82	1482.7570	33.8025	1498.2278	1.0584	1464.3917	18.9042
v83	1497.9654	0.9762	1500.2009	55.1546	1493.3903	2.0167
v84	1511.1134	2.6919	1509.4738	11.2265	1516.8585	2.1352
v85	1536.4027	90.2364	1535.8756	94.8642	1533.3470	63.2342
v86	1639.4243	22.9254	1640.2174	21.0433	1642.7876	9.3241
v87	1652.0902	53.7966	1652.5118	60.2297	1645.9089	31.5320
v88	2639.1174	85.4768	2624.7464	112.3120	2630.3630	112.1330
v89	2790.3892	67.8619	2797.0305	94.7246	2798.1877	108.4010
v90	2994.5223	13.4800	2973.9287	15.6707	2991.2946	5.1797
v91	2998.5439	13.4531	2994.3092	62.1259	2994.3116	12.8598
v92	3002.1965	8.6184	3014.6671	17.5287	2997.8852	17.4617
v93	3017.7235	82.6459	3045.0698	13.3978	3013.2004	89.0868
v94	3059.9383	34.3323	3050.5884	43.4810	3054.0940	27.5627
v95	3067.4273	22.2124	3069.2925	45.2374	3066.7923	28.5408
v96	3107.8834	28.5074	3105.0741	33.4912	3124.2156	24.9460
v97	3187.0243	0.8198	3184.4272	0.9981	3186.3905	0.5525
v98	3194.9519	9.9912	3192.9322	13.9028	3194.7999	8.8786
v99	3207.4056	20.9224	3207.2688	28.0137	3204.9266	20.7152
v100	3214.6635	11.2120	3216.8002	7.3058	3212.4794	12.7499
v101	3229.9225	0.8789	3224.9748	4.3802	3219.9833	2.8205
v102	3576.5599	356.3304	3461.0100	580.0330	3533.9013	552.1934
v103	3713.0827	60.6104	3542.6259	289.5111	3708.1848	80.3709
v104	3730.5330	52.7541	3688.2758	57.1460	3710.5711	33.9024
v105	3749.9918	40.1277	3714.2981	52.4826	3739.9887	39.9469

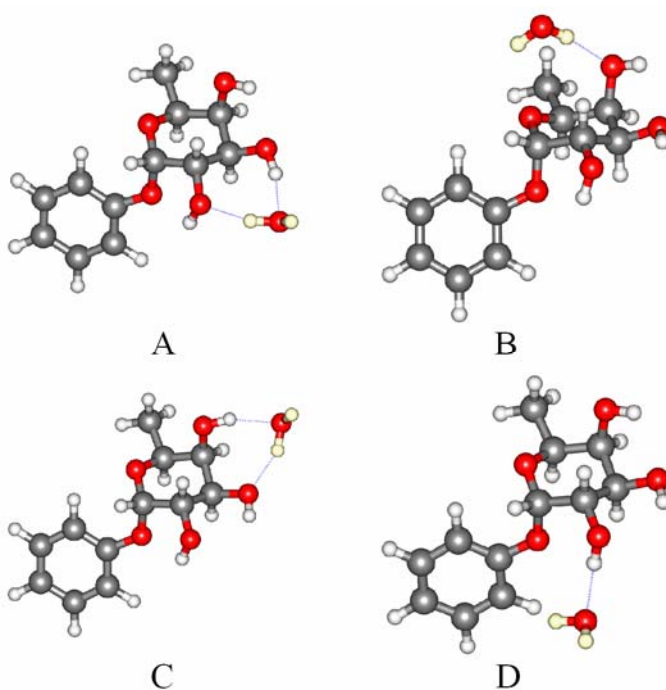
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	21.6978	0.2647	26.3218	0.2178	27.6446	0.0837
v2	25.1583	0.0752	42.7049	0.5265	47.7467	1.6228
v3	37.7447	0.8086	51.7707	0.5718	55.3098	2.4011
v4	52.1753	1.8380	59.3964	1.9472	58.9529	0.3063
v5	81.5394	1.7946	85.7677	0.8495	66.9675	3.2424
v6	101.9138	1.9318	107.9354	7.3966	94.7363	1.7356
v7	111.7754	10.6724	112.6228	4.0629	111.6054	6.4905
v8	130.4147	6.1171	135.1094	6.4536	122.0660	5.0624
v9	141.3930	3.1119	156.4257	4.9309	136.6631	67.2715
v10	160.4934	5.0907	158.7793	7.5034	142.5890	0.8352
v11	179.2982	12.1261	179.6508	8.1035	178.3171	1.9617
v12	182.2660	46.2527	198.4647	76.2084	198.7161	3.4595
v13	211.1858	4.7946	214.3718	31.0002	222.3936	2.0210
v14	228.8382	9.2801	230.2939	21.4647	234.5581	4.1353
v15	253.4951	15.9875	251.3792	6.0591	257.0625	16.9233
v16	264.8906	47.8188	260.4746	4.1097	265.7721	6.6273
v17	292.5628	12.7568	271.0634	11.1533	277.1748	90.8686
v18	304.7987	3.2853	300.7439	8.8155	284.8996	26.9676
v19	340.7636	10.4952	315.7784	0.5188	316.5194	0.9414
v20	383.5749	83.2622	356.2028	8.5371	349.7060	31.7571
v21	385.0212	7.3292	390.1533	57.7634	376.6456	80.2479
v22	393.6868	96.8920	397.5746	62.7131	393.3976	38.9209
v23	407.9749	49.9008	423.8621	0.9168	409.3647	74.1230
v24	424.7908	0.2076	424.7917	30.7811	419.6276	63.0545
v25	435.7126	5.7983	439.0323	198.6753	425.3229	6.9558
v26	443.1624	88.7507	458.2530	87.7166	441.7473	80.4997
v27	461.7196	105.7770	466.5304	30.4990	452.1650	82.2797
v28	472.4844	29.9813	475.5450	15.2830	480.1938	31.0105
v29	478.0544	22.6448	512.9907	25.1008	514.2852	12.9940
v30	524.1185	6.6397	524.9017	10.6802	521.6267	8.8260
v31	575.5700	4.1256	582.5021	6.5394	579.2352	19.7088
v32	605.5006	0.7540	603.7293	2.0017	591.3291	87.8312
v33	629.3461	2.7144	628.9535	2.3281	610.3061	8.5560
v34	630.3552	5.5845	640.4912	2.2262	627.9652	3.4350
v35	696.7824	33.8441	696.0258	25.9061	636.6416	1.2866
v36	707.7918	35.1467	707.8612	27.5659	698.1625	67.9594
v37	755.8321	158.5425	742.8201	159.7286	701.4643	13.0762
v38	779.3452	33.5582	772.0661	56.6555	766.4748	70.4984
v39	788.7338	29.7263	783.6011	24.3374	779.5691	33.5572
v40	838.4842	21.5330	832.7687	22.8825	831.0436	22.0632
v41	848.0135	0.4047	842.8892	0.7735	847.4947	0.2469
v42	878.4120	16.4334	879.4458	16.5041	881.9549	17.6527
v43	898.2291	19.4478	898.4125	21.9576	898.2502	37.0551
v44	929.3819	7.4103	916.0418	4.5234	919.0261	3.3221
v45	958.4700	20.9556	958.0850	20.6348	959.4740	26.0491
v46	978.5958	0.1425	975.2478	0.1625	978.5388	0.0084
v47	999.8916	0.9049	997.1410	0.1305	997.6965	0.1516
v48	1017.2730	15.2599	1014.8691	4.7768	1012.4528	0.5519
v49	1035.3527	15.1199	1036.1854	6.6290	1030.9205	26.2564
v50	1042.1069	87.1781	1045.2257	42.6024	1042.7082	5.1878
v51	1048.5781	89.5956	1057.7040	41.4666	1055.8815	20.4972
v52	1067.0148	154.7014	1059.9384	225.6390	1058.1017	87.7728
v53	1082.4746	131.3464	1081.1932	139.6500	1078.3405	159.0871
v54	1095.6683	138.0177	1096.6704	118.8765	1094.0669	158.9030
v55	1100.7891	26.5165	1103.8081	108.3336	1099.2145	134.7844
v56	1103.4674	143.1318	1107.7889	79.0534	1109.1797	80.7014
v57	1110.1179	12.2081	1115.6162	55.8596	1117.5625	117.7635
v58	1137.3182	61.3364	1137.4852	60.6889	1139.9151	73.8432
v59	1143.6071	44.0785	1147.2674	37.1609	1147.0113	9.4625
v60	1153.8124	3.6034	1154.7896	4.4777	1159.3292	3.2235
v61	1189.3780	0.6136	1190.6236	0.5454	1186.7628	2.7625
v62	1191.7789	18.3101	1207.2044	12.4981	1211.3412	14.6797
v63	1220.2223	4.9254	1214.8592	69.7184	1216.5922	99.4808
v64	1226.4757	102.0534	1225.8029	76.9252	1230.8378	50.8143
v65	1233.2490	87.6367	1236.2830	80.6173	1235.0266	22.0252
v66	1244.1901	136.5507	1250.8173	226.8518	1252.1704	149.7859
v67	1262.2582	26.6061	1263.3787	19.7352	1261.2827	239.3558
v68	1279.7132	2.4863	1280.1205	2.2731	1270.8549	18.6545
v69	1307.1858	23.2640	1309.1776	24.2280	1311.0188	29.4539
v70	1322.8626	22.3878	1322.6267	20.1874	1323.7809	20.4598
v71	1334.7725	0.3125	1346.3535	2.1664	1347.7672	11.0572
v72	1357.5466	1.4938	1367.4715	22.0645	1360.5103	25.0426
v73	1363.9167	9.6045	1368.6796	1.2877	1370.6732	0.4029
v74	1372.2766	18.9404	1376.0565	16.3562	1373.2630	18.1250
v75	1391.4064	5.2601	1394.9087	5.1620	1379.6576	3.5595

v76	1398.3884	9.0714	1400.1433	10.2342	1400.4339	4.4249
v77	1413.4372	19.7249	1416.8865	15.1748	1411.5985	52.4386
v78	1422.2221	104.4755	1421.5229	110.8513	1424.8117	16.4276
v79	1427.9313	13.0675	1430.1408	8.9306	1431.0914	6.3167
v80	1437.6044	2.8143	1437.1053	5.6708	1440.2031	21.5268
v81	1448.1607	15.9122	1446.1457	14.2247	1443.4316	29.5366
v82	1478.0545	21.6190	1464.3075	19.8024	1452.1048	20.7325
v83	1493.3733	2.2488	1499.0596	0.6460	1498.2684	1.5191
v84	1516.6848	2.1820	1515.5880	1.8526	1516.8970	1.9152
v85	1533.1578	65.3904	1536.7784	93.5938	1537.0191	85.5808
v86	1641.9282	10.0278	1641.7784	21.4477	1640.7170	29.0928
v87	1646.2733	33.8008	1651.6975	53.7864	1651.7941	48.1608
v88	2631.0247	109.2306	2633.4718	93.8526	2569.2667	167.5705
v89	2798.4800	98.4875	2798.1561	107.0605	2792.0476	65.8237
v90	2989.6598	6.9691	2989.5842	4.5153	2995.4231	32.8705
v91	2992.4158	10.1816	2995.3371	18.5947	3004.1262	8.1364
v92	2996.0649	18.8555	3000.1037	13.8791	3013.8699	12.5932
v93	3011.6438	97.8247	3013.5479	88.8253	3025.4501	47.4901
v94	3062.4497	17.8842	3056.3525	28.8264	3063.9655	25.7493
v95	3067.7393	28.5450	3071.7536	26.2709	3087.4887	22.0476
v96	3124.6548	24.7009	3127.5505	22.8279	3141.3545	16.6012
v97	3185.8967	1.1780	3186.6503	0.5857	3183.5848	0.6678
v98	3193.8998	7.2861	3194.7536	11.5706	3192.8507	14.4201
v99	3203.1780	19.3889	3206.6246	18.4147	3204.3729	28.4714
v100	3211.3817	15.6324	3213.9631	12.3927	3211.7182	12.8945
v101	3220.2513	2.5537	3233.8384	1.0357	3226.9272	5.0298
v102	3531.7297	551.3139	3560.6940	426.2298	3708.8933	64.9937
v103	3706.8123	78.8302	3706.1452	85.4968	3726.4533	47.0130
v104	3709.7858	36.7949	3708.4513	30.2741	3730.1458	54.7280
v105	3740.0109	38.1456	3746.1662	31.6063	3746.6598	43.2525

Table 9. α -PhFuc $\cdot$ D₂O

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	0.00	0.00
B	11.82	1.60
C	4.19	2.11
D	12.95	4.30



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	-0.014158	0.091502	-0.851298
6	-1.382406	-0.604828	-0.752726
6	-2.142106	-0.184423	0.517195
6	-2.157155	1.348845	0.649759
6	-0.749364	1.933082	0.512231
8	-0.103649	1.472805	-0.699969
8	-1.197642	-2.027721	-0.841287
8	-3.506636	-0.578637	0.486871
8	-3.009989	1.919556	-0.333786
1	-0.433759	-2.242867	-0.275516
1	-3.589477	-1.558625	0.479561
1	0.437315	-0.079918	-1.834121
1	-1.971812	-0.319788	-1.627145
1	-1.635200	-0.610409	1.396388
1	-2.528763	1.597211	1.657486
1	-0.158915	1.575451	1.367764
1	-3.820605	1.380173	-0.333807
1	-1.289530	3.818173	-0.394609
1	0.309652	3.808659	0.394300
8	0.800116	-0.537579	0.150522
6	2.848776	0.502282	-0.718325
6	2.177200	-0.423322	0.087626
6	2.894683	-1.300456	0.910103
6	4.288092	-1.259465	0.917448
6	4.974294	-0.349659	0.105061
6	4.248482	0.523785	-0.706229
1	2.298528	1.213501	-1.323186
1	2.349927	-2.003615	1.534001
1	4.838562	-1.943955	1.557795
1	6.060247	-0.320019	0.110078
1	4.768468	1.243330	-1.333627
6	-0.723162	3.453063	0.465878
1	-1.170975	3.864434	1.377588
8	-3.405137	-3.358870	0.145974
1	-4.043875	-3.782952	-0.445745
1	-2.615370	-3.137648	-0.394132

B			
6	-0.078790	0.171988	0.687662
6	-1.231984	1.183250	0.738498
6	-1.920834	1.289119	-0.625852
6	-2.338146	-0.093021	-1.139210
6	-1.139123	-1.048569	-1.112437
8	-0.510240	-1.071889	0.192842
8	-0.806749	2.464881	1.192166
8	-3.103988	2.081650	-0.537274
8	-3.404666	-0.619814	-0.347883
1	0.007948	2.689844	0.709183
1	-2.899243	2.858916	0.010916
1	0.314385	-0.024142	1.690089
1	-1.950493	0.824732	1.480311
1	-1.224826	1.737408	-1.350658
1	-2.676244	0.000729	-2.182685
1	-0.405225	-0.664923	-1.834799
1	-4.039509	0.108223	-0.218825
1	-2.213567	-2.897766	-0.747421
1	-0.589307	-3.106371	-1.446836
8	0.937009	0.772934	-0.113502
6	3.217906	1.149453	-0.570214
6	2.237695	0.303191	-0.039141
6	2.588822	-0.935619	0.506842
6	3.937860	-1.308489	0.533362
6	4.924719	-0.470797	0.011885
6	4.556109	0.759289	-0.544495
1	2.918480	2.104121	-0.993477
1	1.829871	-1.611943	0.882576
1	4.209523	-2.270810	0.959640
1	5.968180	-0.772143	0.034025
1	5.313133	1.421745	-0.956202
6	-1.491838	-2.487469	-1.458598
1	-1.931731	-2.533981	-2.461100
8	-2.770855	-1.801526	2.244886
1	-1.862313	-2.088135	2.066274
1	-3.067521	-1.459346	1.379294

C			
6	-0.194583	-0.158688	0.851376
6	1.041690	-1.067496	0.796822
6	1.844521	-0.796206	-0.475244
6	2.226460	0.691512	-0.545739
6	0.921800	1.508683	-0.505935
8	0.138164	1.185698	0.670728
8	0.700577	-2.450264	0.897507
8	3.011778	-1.629611	-0.506334
8	3.059929	1.091757	0.524492
1	-0.072369	-2.595943	0.323419
1	2.732620	-2.511329	-0.201109
1	-0.686089	-0.220623	1.827682
1	1.667344	-0.841304	1.663543
1	1.226727	-1.034261	-1.353871
1	2.716662	0.886403	-1.513054
1	0.329148	1.242132	-1.392728
1	3.974494	0.788870	0.337920
1	1.729328	3.285760	0.415036
1	0.191700	3.537225	-0.454376
8	-1.087404	-0.664268	-0.150868
6	-2.934445	0.749738	0.633650
6	-2.427183	-0.326086	-0.103462
6	-3.283433	-1.128094	-0.867781
6	-4.651562	-0.860465	-0.885815
6	-5.175116	0.202835	-0.141627
6	-4.311654	0.999206	0.612231
1	-2.271123	1.399434	1.192688
1	-2.865001	-1.953294	-1.437304
1	-5.310447	-1.488567	-1.479958
1	-6.241738	0.408862	-0.154227
1	-4.703538	1.835018	1.186394
6	1.151338	3.010640	-0.470538
1	1.706290	3.326640	-1.361428
8	5.402585	-0.225660	-0.301259
1	6.059022	-0.516764	0.348391
1	4.764947	-0.962948	-0.408764

D			
6	-0.322810	-0.036781	0.889182
6	-1.504007	0.937201	0.802492
6	-2.237038	0.755341	-0.529656
6	-2.662422	-0.708725	-0.709214
6	-1.456262	-1.639635	-0.513931
8	-0.744419	-1.360485	0.717231
8	-1.157271	2.291891	1.033826
8	-3.419766	1.555453	-0.560990
8	-3.690567	-1.048061	0.212238
1	-0.407987	2.568892	0.461313
1	-3.193501	2.410428	-0.153924
1	0.146047	0.010753	1.877103
1	-2.188026	0.664185	1.611587
1	-1.573517	1.042297	-1.358133
1	-3.026373	-0.847744	-1.740975
1	-0.767620	-1.456512	-1.351070
1	-4.316448	-0.302469	0.209584
1	-2.507349	-3.308609	0.367627
1	-0.932430	-3.725755	-0.356659
8	0.623193	0.370196	-0.106976
6	2.390771	-1.042563	0.853247
6	1.919336	-0.088453	-0.057166
6	2.789975	0.471103	-1.004972
6	4.134492	0.098794	-1.021251
6	4.621887	-0.833903	-0.099712
6	3.743140	-1.400453	0.825988
1	1.717294	-1.523823	1.552612
1	2.392566	1.169579	-1.737594
1	4.799875	0.536063	-1.761428
1	5.668610	-1.124092	-0.112500
1	4.104236	-2.141471	1.534742
6	-1.832325	-3.112676	-0.469327
1	-2.336968	-3.400994	-1.398525
8	1.103317	3.446652	-0.241322
1	1.382576	4.200057	0.301282
1	1.814691	2.788552	-0.171161

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	31.5300	0.1163	26.2090	9.0329	27.6334	0.8435
v2	39.9982	1.4738	29.6393	0.3064	38.2972	0.9021
v3	46.2994	0.0807	47.2699	0.2803	48.3731	0.0566
v4	60.5329	0.6188	48.8392	4.5610	60.3513	6.8109
v5	113.4271	10.1475	66.7918	1.2710	114.0431	6.9752
v6	127.3111	9.0312	101.4725	4.3626	126.5613	0.9203
v7	134.9102	0.1324	131.5753	1.6902	135.0836	2.7764
v8	148.4875	7.1858	140.1196	2.5110	144.1376	4.5286
v9	157.5038	0.2893	180.6905	8.0152	175.9998	3.0128
v10	207.3929	58.2536	183.8009	10.4133	199.5309	1.837
v11	217.7733	19.8745	201.4579	6.6808	205.6859	71.4307
v12	224.4691	3.8152	221.8654	25.4421	215.6936	2.3318
v13	243.0968	34.5653	227.6441	15.5829	250.3226	8.9143
v14	265.9000	8.2844	239.2445	27.3362	257.1983	0.5583
v15	276.8842	63.3282	258.9360	6.6098	268.8050	37.4946
v16	280.8657	3.8307	273.3772	6.4911	285.9871	6.2993
v17	306.8342	5.5234	274.8464	0.6700	298.0299	1.5321
v18	344.1597	25.3006	296.7793	15.4840	323.1574	16.8432
v19	359.5193	0.7336	359.8474	5.7091	358.8877	14.1395
v20	393.2395	4.5142	379.7710	6.6145	378.0652	4.6893
v21	413.1081	7.5785	400.2304	43.4014	401.3177	27.6646
v22	422.1554	0.2845	418.3136	44.1892	420.6169	10.9907
v23	443.2367	21.1158	420.4860	4.9466	424.3379	4.1291
v24	464.9563	161.1565	423.9679	2.3555	431.2921	60.3448
v25	494.9120	27.1716	439.7832	6.5695	452.1064	74.1623
v26	518.2966	4.2107	492.8134	185.6379	511.8503	83.0527
v27	535.0907	17.6257	517.3922	11.7320	523.7282	82.6268
v28	551.4431	50.1812	523.7751	104.7384	532.6819	15.7388
v29	553.4935	47.7175	534.4386	43.3503	558.2378	22.9201
v30	627.2353	1.4944	556.9375	18.0920	626.8541	1.614
v31	653.6538	16.1855	626.9606	1.4177	647.3787	13.8711
v32	681.9423	40.6911	649.1243	15.3847	677.5577	30.9862
v33	699.8317	20.3525	682.8670	38.3282	700.6788	22.4602
v34	706.8867	3.4716	700.8376	21.4817	708.7853	8.0061
v35	750.8970	89.4024	710.7981	4.3133	748.2549	32.2035
v36	764.2766	64.2565	759.4093	25.6675	763.0672	159.2794
v37	768.4777	48.0200	767.5247	55.3831	767.6811	19.5994
v38	799.7034	15.6048	794.5869	10.6713	795.8562	15.0726
v39	836.7387	0.4297	836.4182	0.2563	838.4914	0.355
v40	865.0579	62.0664	861.9409	57.2828	857.5186	59.1754
v41	894.3839	23.7438	893.1081	19.9938	896.7804	28.7994
v42	906.2445	11.2256	907.6267	9.6515	908.3233	10.7472
v43	926.2630	13.8000	927.9301	3.8621	920.9112	7.3317
v44	971.0621	0.0472	971.7615	0.1470	971.9772	9.3579
v45	977.1067	113.6676	981.7934	102.0188	973.6009	74.7149
v46	992.7506	0.1313	994.2443	0.4102	992.9606	0.3124
v47	1005.9690	13.5886	1009.6465	12.3737	1008.4739	28.417
v48	1014.8898	0.3711	1015.6226	2.5193	1015.0747	0.8805
v49	1031.3664	116.6292	1028.9889	176.2032	1025.7120	169.0446
v50	1051.4886	5.3289	1050.8828	1.9166	1051.6490	1.4977
v51	1058.2936	84.3918	1055.5293	110.8016	1055.5312	87.7698
v52	1075.0764	206.7297	1091.6342	285.0387	1090.9884	270.9385
v53	1109.4940	21.2339	1109.1200	16.5985	1108.8365	26.8152
v54	1115.4300	111.1904	1112.9115	118.2026	1113.8912	112.2388
v55	1140.4186	119.5768	1129.4213	20.9556	1136.9568	91.4383
v56	1147.7243	81.7394	1146.5715	13.2277	1148.0309	25.953
v57	1171.7446	10.9287	1158.2823	10.8590	1163.0399	21.3903
v58	1188.0118	3.7094	1180.5287	47.0532	1180.9399	20.0277
v59	1189.9740	19.7962	1188.4918	3.9531	1188.0645	2.9378
v60	1205.4907	18.6954	1205.6302	18.6049	1206.1276	13.9703
v61	1220.7933	59.1125	1224.8012	7.7669	1228.1311	49.7613
v62	1234.7318	45.9835	1249.4930	249.5565	1237.2109	2.6868
v63	1253.8966	238.3934	1251.2429	139.4943	1254.0093	304.7423
v64	1267.9307	104.5508	1268.7466	15.7787	1276.9076	26.6294
v65	1295.5427	21.6532	1277.3387	111.5999	1299.5681	77.7359
v66	1312.6468	10.2851	1319.9164	7.5346	1321.4639	14.1214
v67	1344.7472	23.2110	1344.9432	23.7571	1343.4684	24.3567
v68	1346.2728	1.6467	1349.2709	10.6254	1347.2003	2.6555
v69	1365.5106	4.8598	1365.8050	5.2245	1366.0765	5.506
v70	1373.1367	51.9003	1371.0788	28.8229	1376.0981	42.8998
v71	1379.0828	4.3156	1377.7753	4.8211	1381.0833	11.9213
v72	1394.2188	28.4511	1393.9547	10.4297	1395.5118	23.6012
v73	1407.3172	4.9093	1402.4715	21.4531	1405.8191	3.637
v74	1426.4900	2.4189	1410.7934	12.7816	1417.0221	10.0138
v75	1434.6689	13.1892	1433.8590	6.8676	1434.1932	22.558

v76	1438.1292	26.5385	1437.7394	17.4725	1436.8729	0.9193
v77	1448.7560	14.3664	1442.4145	19.5405	1448.1583	38.1814
v78	1465.3469	55.7829	1450.4805	23.6314	1481.1368	17.7137
v79	1498.6141	0.4864	1498.4072	0.5879	1498.0798	0.5201
v80	1508.5031	4.1984	1510.8984	4.6215	1508.7561	4.5465
v81	1522.6664	3.6042	1522.3087	3.6258	1519.9525	4.5479
v82	1535.5123	99.5953	1536.1338	97.6779	1536.3465	101.5828
v83	1638.8030	23.9630	1640.0458	23.6455	1638.9544	23.0212
v84	1651.8537	65.0328	1652.1168	60.9241	1651.9271	67.3832
v85	2572.6637	194.1199	2637.6788	115.4290	2594.3807	149.2964
v86	2790.9310	100.0309	2783.7477	42.8875	2795.0936	93.9783
v87	2994.3206	36.7627	3012.7277	25.5518	3004.8411	27.1547
v88	3019.9880	17.7842	3025.3318	21.5896	3021.1762	8.3109
v89	3036.0652	47.4871	3042.4996	45.5663	3036.0951	57.4312
v90	3063.3181	25.5410	3064.6533	20.9447	3062.3537	26.3936
v91	3088.2895	21.6622	3097.2874	17.1277	3093.2097	21.1663
v92	3126.8515	23.2188	3122.5368	3.6341	3124.9580	24.371
v93	3129.1836	9.7194	3129.6326	18.9530	3128.7507	7.5012
v94	3153.9973	11.1680	3150.7996	12.2465	3155.9917	10.6326
v95	3184.4031	1.7377	3185.4563	1.5047	3183.6923	1.72
v96	3192.0269	10.5356	3193.1911	9.7022	3191.4347	10.9654
v97	3203.5332	23.9596	3204.5703	23.3224	3203.2153	25.4482
v98	3211.9431	15.7962	3212.6954	14.7568	3211.4498	15.8785
v99	3235.2641	0.8361	3234.9882	1.2366	3235.0275	0.6554
v100	3507.0789	684.9790	3693.9677	78.3338	3544.4403	636.4242
v101	3691.9600	81.9042	3708.2328	45.6596	3697.9356	66.0834
v102	3703.0660	61.0989	3716.5893	51.5719	3703.9685	47.5983

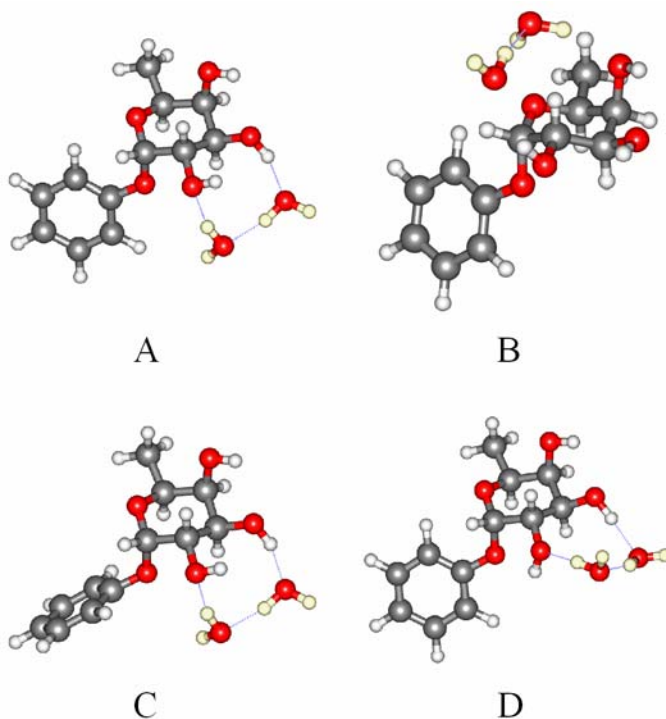
D		
	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	20.1265	1.1977
v2	33.8973	1.9195
v3	46.8083	2.1485
v4	62.3468	1.6602
v5	83.6803	1.2259
v6	94.6515	17.2661
v7	119.2477	2.1596
v8	129.8250	33.4085
v9	147.7768	14.4857
v10	163.3607	7.2229
v11	193.3391	20.3870
v12	224.4702	7.7692
v13	233.1725	7.8380
v14	248.2592	39.1440
v15	259.7548	65.4044
v16	271.1496	13.4536
v17	277.7928	4.3201
v18	293.4907	6.1109
v19	296.8689	7.1388
v20	367.1249	4.7256
v21	378.0999	8.1197
v22	421.6343	5.1985
v23	425.0194	1.3423
v24	435.1069	15.8995
v25	454.4135	42.1150
v26	471.7035	137.0420
v27	520.0214	6.6099
v28	533.7844	8.4742
v29	557.7576	6.3328
v30	626.9253	1.8375
v31	645.4343	17.2703
v32	685.0010	42.8634
v33	703.5789	18.1874
v34	709.2301	4.0818
v35	742.9583	119.0573
v36	760.9138	28.7269
v37	765.3113	80.9915
v38	792.9354	22.8695
v39	840.1229	2.6070
v40	861.1771	51.9938
v41	894.9542	17.6449
v42	904.9158	10.0534
v43	930.0451	15.5737
v44	972.7863	0.8556
v45	977.5541	116.4543
v46	993.1714	0.1244
v47	1007.3473	14.0968
v48	1013.3370	2.1726
v49	1030.3543	173.6550
v50	1052.6929	8.9330
v51	1059.7694	65.5486
v52	1106.3559	170.1751
v53	1111.4267	11.1057
v54	1117.3217	249.0099
v55	1141.3611	23.8741
v56	1145.1107	19.3078
v57	1164.5160	5.0149
v58	1180.4132	48.1176
v59	1188.0985	3.1252
v60	1208.5590	22.0433
v61	1224.7847	23.0324
v62	1235.8930	31.9216
v63	1260.4915	319.7675
v64	1267.5489	17.4569
v65	1301.3657	64.1513
v66	1326.7707	22.9922
v67	1348.6586	10.7499
v68	1349.4004	21.2893
v69	1367.4528	7.8412
v70	1374.9272	13.7963
v71	1378.7021	11.5397
v72	1392.2387	19.1600
v73	1399.5423	23.4468
v74	1408.1958	20.5187
v75	1434.9296	13.4606

v76	1440.5103	12.7193
v77	1442.1269	21.4965
v78	1455.0728	42.2464
v79	1497.9073	0.5278
v80	1509.5788	4.5050
v81	1522.2669	4.1068
v82	1536.4313	99.0999
v83	1637.1124	20.6899
v84	1650.6746	79.4027
v85	2682.2026	24.4740
v86	2815.1827	88.5574
v87	2988.2997	42.8954
v88	3028.0829	3.2983
v89	3037.5817	56.5259
v90	3062.5217	25.9855
v91	3093.2375	21.4977
v92	3106.5486	20.4510
v93	3126.0617	23.2099
v94	3153.2901	11.3826
v95	3182.2959	3.9319
v96	3189.5030	4.6329
v97	3198.0841	19.2236
v98	3210.9397	20.5058
v99	3237.4591	1.5579
v100	3538.2713	437.4713
v101	3702.9787	90.4337
v102	3705.1372	22.4766

Table 10. α -PhFuc $\cdot$ (D₂O)₂

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	2.57	0.00
B	13.26	0.21
C	6.52	3.01
D	0.00	3.38



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.145683	-0.529372	0.987062
6	-1.266069	0.015772	1.197344
6	-2.068907	-0.030325	-0.103705
6	-2.084939	-1.466869	-0.650306
6	-0.657589	-2.028511	-0.732109
8	0.074721	-1.845194	0.504723
8	-1.199589	1.343813	1.734124
8	-3.402517	0.399624	0.167088
8	-2.892760	-2.297761	0.174871
1	-2.106787	1.574801	1.997889
1	-3.567331	1.223865	-0.346832
1	0.691551	-0.583561	1.934485
1	-1.745828	-0.642915	1.930142
1	-1.603041	0.630250	-0.844113
1	-2.493799	-1.448891	-1.674167
1	-0.136505	-1.464809	-1.519116
1	-3.720930	-1.808537	0.324949
1	-1.110750	-4.088679	-0.262577
1	0.432017	-3.848418	-1.123553
8	0.826574	0.357039	0.101845
6	2.823107	1.362952	-0.636112
6	2.201772	0.286952	0.010751
6	2.970019	-0.774253	0.505026
6	4.362031	-0.732253	0.364862
6	4.989630	0.339567	-0.271587
6	4.209545	1.385700	-0.777017
1	2.208622	2.171228	-1.022270
1	2.495928	-1.633913	0.963767
1	4.953989	-1.558174	0.751341
1	6.070562	0.359043	-0.378534
1	4.681625	2.226477	-1.278974
6	-0.608126	-3.516018	-1.046153
1	-1.109866	-3.716808	-1.999672
8	-3.304442	2.780885	-1.226548
1	-2.465734	3.168519	-0.872329
1	-3.970276	3.483130	-1.198808
8	-0.934797	3.488196	-0.021713
1	-0.114755	3.543144	-0.534032
1	-0.823126	2.721364	0.588950

B			
6	-0.019257	-0.358867	0.231656
6	1.207798	-1.020127	-0.409756
6	1.703509	-0.183019	-1.583649
6	2.045320	1.223656	-1.067117
6	0.852979	1.829922	-0.312941
8	0.351294	0.932408	0.707890
8	0.993662	-2.360881	-0.817757
8	2.903914	-0.735288	-2.125628
8	3.192527	1.162617	-0.205957
1	1.194688	-2.910250	-0.036352
1	2.775134	-1.699667	-2.165027
1	-0.344828	-0.915301	1.116309
1	1.989134	-1.003580	0.348718
1	0.935009	-0.115625	-2.364686
1	2.277620	1.876895	-1.921392
1	0.052340	1.979684	-1.049992
1	3.839602	0.601787	-0.672475
1	1.490808	3.890862	-0.373506
1	0.273847	3.535742	0.871274
8	-1.058500	-0.306934	-0.721048
6	-3.346950	-0.539786	-1.215043
6	-2.363240	-0.151853	-0.297244
6	-2.724391	0.374885	0.947969
6	-4.081513	0.491843	1.270947
6	-5.070141	0.105569	0.364718
6	-4.694067	-0.407254	-0.882461
1	-3.037099	-0.949145	-2.171988
1	-1.966871	0.713295	1.645763
1	-4.359749	0.900314	2.239351
1	-6.120735	0.204524	0.623392
1	-5.453012	-0.713589	-1.597957
6	1.168092	3.152972	0.369618
1	1.967993	3.038537	1.106434
8	2.592590	0.057046	2.491502
1	3.048877	0.420582	1.705314
1	1.709875	0.459723	2.403028
8	1.930736	-2.665216	2.015749
1	2.144298	-3.302742	2.712373
1	2.264442	-1.789705	2.323227

C			
6	-0.125136	0.477017	0.953731
6	1.217464	-0.213436	1.185149
6	2.100291	-0.106037	-0.058114
6	2.288389	1.372555	-0.425061
6	0.923731	2.071202	-0.536117
8	0.075037	1.819721	0.609384
8	0.990240	-1.578882	1.560207
8	3.363963	-0.708080	0.220968
8	3.100049	2.024534	0.544852
1	1.860366	-1.943619	1.797574
1	3.466277	-1.480575	-0.380712
1	-0.728025	0.493195	1.866055
1	1.707151	0.310604	2.013791
1	1.616447	-0.621951	-0.894922
1	2.771433	1.432044	-1.414412
1	0.427435	1.649814	-1.422229
1	3.875884	1.452724	0.680504
1	1.616357	3.842959	-1.558640
1	0.025893	4.016875	-0.779042
8	-0.821620	-0.254252	-0.064731
6	-2.962488	-0.755807	0.942894
6	-2.206529	-0.163062	-0.073673
6	-2.833198	0.467743	-1.150233
6	-4.228901	0.508185	-1.207824
6	-4.994548	-0.070417	-0.191255
6	-4.357305	-0.700781	0.882071
1	-2.460127	-1.265870	1.760377
1	-2.224216	0.918257	-1.928326
1	-4.716897	0.998867	-2.046115
1	-6.079605	-0.034243	-0.236710
1	-4.945892	-1.162177	1.670945
6	1.025245	3.582816	-0.673037
1	1.510353	4.013787	0.206413
8	3.017254	-2.870361	-1.471772
1	2.094061	-3.148661	-1.245919
1	3.545515	-3.678581	-1.540568
8	0.447772	-3.300007	-0.582928
1	0.455206	-2.675240	0.179576
1	-0.281261	-2.999491	-1.146671

D			
6	0.308046	0.307343	-0.863925
6	-1.171169	-0.105771	-0.800374
6	-1.864960	0.454018	0.451983
6	-1.586563	1.962903	0.583390
6	-0.092019	2.273030	0.466855
8	0.480751	1.683863	-0.725353
8	-1.272316	-1.532889	-0.897641
8	-3.274168	0.307422	0.364855
8	-2.304640	2.678427	-0.414531
1	-0.625814	-1.909867	-0.274233
1	-3.564658	-0.544196	0.768058
1	0.745791	0.041220	-1.831721
1	-1.672577	0.293966	-1.684519
1	-1.476143	-0.059249	1.342932
1	-1.919661	2.283484	1.584427
1	0.405301	1.824841	1.339042
1	-3.206239	2.310791	-0.411480
1	-0.158062	4.259544	1.307727
1	1.300484	3.916886	0.350221
8	0.958431	-0.454324	0.164482
6	3.193264	0.176876	-0.630388
6	2.330109	-0.623641	0.125903
6	2.836608	-1.659585	0.920209
6	4.209107	-1.902510	0.948973
6	5.083240	-1.119840	0.186109
6	4.567757	-0.086201	-0.597463
1	2.809623	1.006226	-1.213113
1	2.146883	-2.262280	1.504516
1	4.595297	-2.709621	1.566258
1	6.152339	-1.311884	0.207479
1	5.236658	0.536426	-1.186316
6	0.218398	3.761066	0.407196
1	-0.256613	4.216071	-0.465628
8	-3.435581	-3.265471	-1.043730
1	-2.687942	-2.631069	-1.139145
1	-3.989509	-3.154153	-1.830321
8	-4.040660	-2.140319	1.373809
1	-3.994505	-2.688919	0.552773
1	-4.926089	-2.258012	1.747110

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	22.4125	0.1462	19.7805	0.5107	22.5699	0.0501
v2	35.9404	1.0220	34.0309	0.3641	24.3165	0.0709
v3	40.7979	0.5321	48.0012	0.0218	38.1047	0.9934
v4	44.7053	2.8782	56.4330	2.2159	47.5636	0.5163
v5	47.8331	0.1336	60.7083	0.2684	50.0639	1.7012
v6	76.8812	3.7636	79.2660	1.7484	75.3220	3.6547
v7	112.0928	9.3155	112.3843	8.8080	105.0162	5.4777
v8	114.5908	5.8145	122.0661	44.4043	117.3106	8.8043
v9	139.5894	3.5538	127.9785	10.7591	137.6445	3.2319
v10	166.4671	37.5867	136.3916	9.7626	155.5600	5.4366
v11	180.0490	5.5258	146.1322	5.0001	173.3490	31.5645
v12	189.3733	5.4105	157.3747	7.7129	192.9777	4.5001
v13	202.1573	15.7462	178.8536	5.3232	216.8088	16.5778
v14	218.1611	36.6769	198.4220	17.1781	219.4127	4.3129
v15	226.5075	0.8959	205.3048	13.5181	226.0682	6.0559
v16	236.1531	53.3455	219.0975	1.9729	234.1126	78.0887
v17	247.4953	12.7574	242.2262	23.0317	245.4210	7.2464
v18	257.9847	30.9390	260.0164	3.8295	254.7923	11.7306
v19	263.5153	9.9588	275.4946	14.8097	261.4322	40.3127
v20	284.0319	19.6988	278.6199	0.3075	285.2782	39.3121
v21	292.2765	32.2751	295.1313	12.0006	297.1114	4.5764
v22	303.3839	12.4523	333.6447	62.2303	318.5836	0.7150
v23	357.2696	21.8843	360.0996	36.6072	366.0956	37.9176
v24	364.3644	13.1059	368.0197	2.4426	378.0272	5.1015
v25	381.3793	5.9754	382.7929	5.0936	398.0547	2.5851
v26	422.3591	0.2754	423.2127	5.3552	424.2612	0.1548
v27	428.6350	2.8352	425.8424	6.6857	432.2722	5.1644
v28	438.5211	14.4476	435.3564	8.6889	437.9406	12.4006
v29	482.5259	105.6096	454.8455	100.7758	472.5247	73.1005
v30	493.9103	68.4271	495.1816	66.1137	477.5844	43.4972
v31	518.6296	4.3843	514.8778	6.9629	501.3635	85.1857
v32	527.1282	83.9813	531.7961	89.6179	543.3239	57.6371
v33	546.3481	13.9529	544.4612	127.2716	550.6099	11.4006
v34	561.1687	45.7709	554.6167	23.3432	562.4364	75.1979
v35	618.5371	74.7454	579.5771	26.3873	626.7633	7.9703
v36	627.7236	4.2516	595.3692	44.7992	632.7077	32.0350
v37	643.8318	16.7055	627.2261	0.6648	640.4934	42.3930
v38	680.6491	44.7593	647.7969	22.5447	665.3259	52.1093
v39	700.6868	24.2020	685.4279	50.9547	702.5052	30.0382
v40	709.9387	3.9539	701.7994	22.5231	711.2969	6.2471
v41	756.0967	82.6453	715.0512	16.9559	750.1065	43.8566
v42	762.4124	3.1795	754.4204	16.8280	756.6195	31.7164
v43	766.6516	55.8444	767.2779	56.9404	779.3368	42.9016
v44	794.7275	14.0315	793.9950	11.5365	799.2730	19.4310
v45	832.8985	0.4852	839.1486	0.4635	843.5504	0.2567
v46	860.5214	56.4116	859.7557	44.9214	864.5734	38.1115
v47	891.9735	12.5444	887.4512	25.6253	892.9380	24.7682
v48	901.8077	5.9319	908.9916	8.6462	910.6680	18.9286
v49	928.8790	8.9711	934.6815	7.4821	930.4871	1.5493
v50	968.4546	0.3182	972.0618	0.6554	970.1033	184.9567
v51	978.6485	110.4301	979.1063	119.9724	974.0388	0.3754
v52	990.9551	0.5030	992.3466	0.5441	996.2376	1.6030
v53	1008.8348	22.2187	1011.0470	25.4402	1002.9300	53.2456
v54	1015.0747	1.9890	1015.3367	4.2206	1017.9494	0.7978
v55	1033.6620	182.9386	1031.5733	307.1601	1029.4493	159.8456
v56	1051.1162	5.6456	1039.3147	17.9329	1048.1332	13.7964
v57	1055.9486	109.5339	1052.1894	29.8066	1052.6873	35.0564
v58	1093.7424	191.1146	1100.3381	94.7894	1094.9161	176.9519
v59	1107.6345	49.0156	1109.1921	50.0618	1101.7870	5.4818
v60	1111.1106	66.3026	1111.9995	42.9686	1112.0786	90.3960
v61	1131.6454	57.2963	1131.9929	105.0776	1136.9053	35.5508
v62	1140.0276	42.1503	1141.5183	23.8673	1137.8046	85.7601
v63	1171.2450	24.5767	1158.8082	4.5665	1170.6243	24.8523
v64	1186.9654	2.9472	1183.5741	43.2512	1188.3175	0.7034
v65	1197.5371	27.6051	1187.5611	6.8723	1193.9866	18.0117
v66	1205.6881	17.6503	1204.4318	20.0149	1199.4729	34.2847
v67	1229.9706	29.3192	1232.2904	35.1212	1231.8898	28.9904
v68	1241.2097	90.9479	1243.4992	125.9271	1237.5249	126.5267
v69	1246.6842	69.6815	1258.1248	326.1364	1245.7962	80.7904
v70	1257.5963	251.3773	1260.9953	49.2141	1249.2861	123.8639
v71	1277.9407	28.8565	1276.3751	47.1163	1276.6420	38.7090
v72	1299.9597	12.9828	1302.3462	12.4502	1299.9022	10.1671
v73	1333.5129	6.5669	1335.8960	4.8439	1330.8677	5.8835
v74	1339.7002	37.1933	1347.0117	43.8081	1333.6744	4.0353
v75	1346.3038	2.1142	1359.0519	14.7870	1343.0767	33.3410

v76	1365.7748	3.8913	1367.0275	16.0736	1358.8978	0.7089
v77	1374.6915	9.6983	1379.4557	23.5610	1368.7865	30.4338
v78	1379.1229	20.7341	1380.0227	0.4262	1379.1277	5.2250
v79	1399.5844	48.0741	1395.7308	4.5983	1402.7484	28.9460
v80	1407.7204	11.4244	1400.5379	16.5433	1411.9243	10.1601
v81	1427.3554	8.0236	1414.6639	56.3121	1426.7747	8.5795
v82	1434.0162	10.0787	1428.1040	7.7443	1433.3663	6.8361
v83	1435.0526	16.2369	1436.6128	13.5020	1434.2844	17.1286
v84	1448.6824	10.5627	1444.1100	13.7471	1446.0395	15.2568
v85	1478.1251	23.0293	1481.5947	10.6590	1478.1346	24.4731
v86	1498.0116	0.5388	1498.0337	0.3664	1493.1309	1.7092
v87	1507.8300	5.0534	1511.3853	4.9511	1506.7767	5.1687
v88	1521.0433	3.9166	1520.4355	3.1744	1520.8404	3.8403
v89	1536.2332	101.4311	1536.5059	102.1497	1534.2913	78.8114
v90	1637.6936	23.0413	1638.3389	21.0529	1639.3069	8.7866
v91	1652.5722	68.0350	1652.4760	69.1557	1647.7752	50.7466
v92	2473.9627	298.6818	2523.6823	214.8126	2465.3180	310.7242
v93	2532.8495	271.6423	2626.8096	97.8582	2542.2974	255.3311
v94	2786.1797	56.7363	2731.4595	59.0761	2778.5113	51.5468
v95	2787.2970	62.7686	2790.6033	61.8296	2788.0606	67.6661
v96	2991.0899	41.2309	3022.8289	28.2134	2991.9213	40.1284
v97	3031.5647	27.8270	3045.2008	14.4433	3028.6808	33.4320
v98	3062.3888	25.1841	3060.2055	34.7158	3061.8693	25.8446
v99	3072.2479	4.4775	3063.6760	25.5846	3074.4154	2.3144
v100	3084.7005	19.6535	3096.4954	17.6452	3087.9592	25.4617
v101	3094.4514	28.6571	3128.7442	19.4134	3106.4872	21.2077
v102	3125.6650	23.6382	3146.1480	16.1165	3125.5739	24.3178
v103	3153.0013	11.5775	3159.0993	5.1775	3152.9306	11.4833
v104	3182.9823	3.0016	3182.7868	1.1238	3183.2037	1.8891
v105	3190.5528	8.8313	3191.0093	15.5876	3190.8947	7.6608
v106	3202.4673	35.3090	3205.9357	28.4977	3201.4383	22.7913
v107	3211.2011	16.2735	3214.2812	8.3269	3208.6614	20.8061
v108	3236.3074	0.8571	3231.4365	2.2189	3214.6545	5.1378
v109	3472.5460	750.8131	3662.6085	162.8495	3489.0107	699.8659
v110	3705.2854	48.4622	3683.8275	76.6041	3708.4284	44.3434
v111	3724.8163	54.0268	3704.8056	53.3903	3721.2143	55.8027

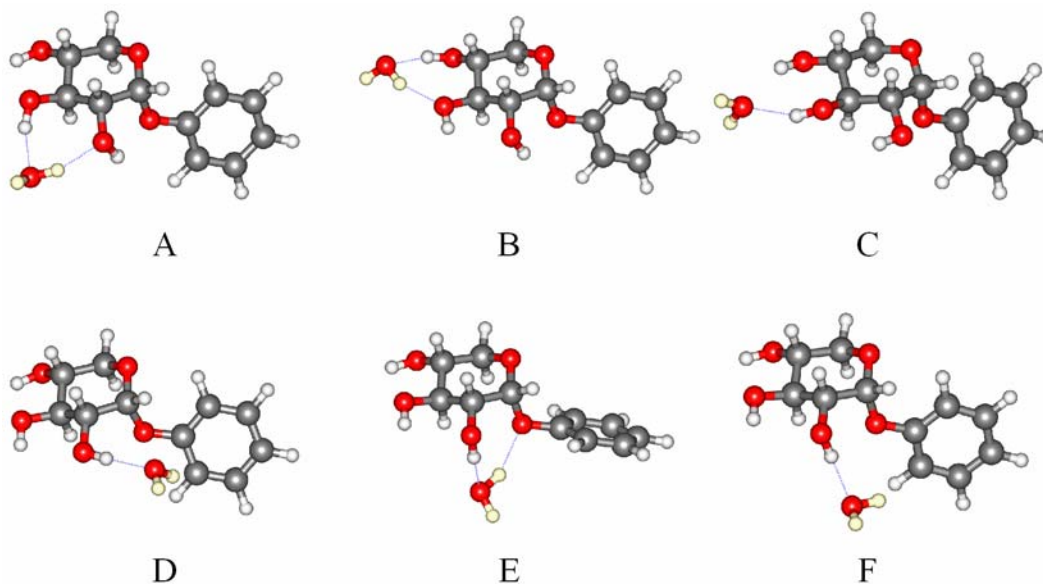
D		
	Frequency / cm ⁻¹	Intensity / km mol ⁻¹
v1	25.5880	3.0431
v2	28.1040	2.2265
v3	32.9387	0.8341
v4	42.5276	1.8443
v5	50.5688	1.5447
v6	70.8942	3.1614
v7	112.8688	10.018
v8	127.2472	11.3411
v9	139.2386	1.3062
v10	148.5151	5.8106
v11	172.9234	15.4778
v12	181.9789	16.8022
v13	192.8937	48.7552
v14	215.7725	3.1101
v15	225.4260	0.9839
v16	243.7932	4.0744
v17	252.8798	18.5928
v18	260.7961	14.2852
v19	278.0526	4.9397
v20	288.8171	6.6168
v21	302.4533	57.2974
v22	323.2008	12.9702
v23	354.9250	8.5844
v24	388.3358	81.0903
v25	398.5859	40.5874
v26	413.9951	6.9134
v27	423.9950	0.145
v28	440.8621	47.2944
v29	474.3657	82.5794
v30	497.7300	130.7302
v31	515.1526	26.3685
v32	520.9171	13.8007
v33	537.8373	4.0816
v34	554.6168	11.1074
v35	569.9391	89.8713
v36	627.0804	1.4506
v37	649.8582	14.7811
v38	681.7688	47.1151
v39	701.2288	20.8077
v40	707.6587	4.1543
v41	762.5627	69.2904
v42	768.6793	23.697
v43	794.4712	9.5761
v44	825.6677	80.4654
v45	839.7528	0.7257
v46	865.3042	56.3663
v47	895.1346	30.8989
v48	909.4661	11.5804
v49	928.7481	14.926
v50	972.7591	0.1058
v51	977.4104	113.6907
v52	993.0929	0.2685
v53	1005.6427	7.8578
v54	1015.0240	0.2879
v55	1033.8960	120.8116
v56	1051.8731	7.1518
v57	1058.4238	68.5571
v58	1084.3503	232.6629
v59	1109.3690	26.3276
v60	1114.7977	124.2
v61	1138.7143	112.7306
v62	1145.9680	62.0879
v63	1169.5400	16.5869
v64	1188.1194	2.6602
v65	1195.2798	26.1819
v66	1205.9081	15.8393
v67	1229.5269	50.0737
v68	1242.7608	74.7695
v69	1255.3155	207.9783
v70	1257.1220	58.4853
v71	1268.7583	94.4745
v72	1299.3891	4.0679
v73	1313.5468	19.6385

v74	1343.9587	24.2737
v75	1345.4565	3.3376
v76	1366.6544	5.3982
v77	1374.4409	52.9518
v78	1380.4032	4.1235
v79	1397.4936	28.3042
v80	1408.5162	2.3084
v81	1419.4417	6.3251
v82	1433.9820	15.3291
v83	1445.0578	28.5484
v84	1447.6431	15.8655
v85	1462.1001	28.3555
v86	1498.0080	0.4782
v87	1509.6755	4.4701
v88	1520.8201	3.5997
v89	1536.3980	100.9614
v90	1638.9565	23.1609
v91	1651.8137	67.9372
v92	2486.6295	235.2053
v93	2550.8336	433.8858
v94	2785.8197	91.8495
v95	2788.3204	67.8686
v96	2990.7889	42.4661
v97	3030.0785	13.381
v98	3041.4116	41.4487
v99	3062.5175	26.6124
v100	3089.8830	22.3088
v101	3125.6413	24.2386
v102	3130.8612	9.4422
v103	3153.4153	11.4846
v104	3183.8475	1.5585
v105	3191.5328	11.3361
v106	3203.4405	25.002
v107	3211.6683	15.226
v108	3235.6782	0.6371
v109	3452.9787	1013.496
v110	3702.8747	71.5453
v111	3705.3743	56.8267

Table 11. α -PhXyl $\cdot$ D₂O

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6- 31+G(d) energy / kJ mol ⁻¹
A	0.00	0.00
B	0.89	0.50
C	20.63	4.95
D	16.13	5.04
E	14.71	5.21
F	13.32	5.22



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.000061	-0.253382	-0.982234
6	-1.395841	0.400333	-0.930942
6	-2.241330	-0.159033	0.226957
6	-2.208965	-1.689048	0.199415
6	-0.769076	-2.189688	0.197426
8	-0.061040	-1.650769	-0.934901
8	-1.250931	1.827979	-0.873076
8	-3.610391	0.207443	0.138795
8	-2.864578	-2.236146	1.333654
1	-0.528912	2.004606	-0.242306
1	-3.716641	1.168748	0.314631
1	0.511369	-0.007596	-1.918650
1	-1.908915	0.189562	-1.873950
1	-1.813708	0.180494	1.183156
1	-2.706488	-2.025030	-0.724355
1	-0.263226	-1.916024	1.131168
1	-0.730061	-3.273805	0.078296
1	-3.721250	-1.780721	1.406328
8	0.724454	0.315446	0.111369
6	2.854529	-0.618082	-0.676910
6	2.108289	0.253571	0.122604
6	2.745894	1.122507	1.015435
6	4.137565	1.128424	1.098920
6	4.899151	0.274265	0.293306
6	4.251303	-0.592508	-0.587998
1	2.362644	-1.324623	-1.335348
1	2.142843	1.781670	1.633603
1	4.627402	1.805964	1.793493
1	5.983563	0.281690	0.357923
1	4.830495	-1.270092	-1.210137
8	-3.501481	3.006393	0.244069
1	-4.135219	3.506572	-0.290982
1	-2.711633	2.851662	-0.318026

B			
6	0.223032	0.155410	-1.038780
6	-1.049634	1.009795	-0.972593
6	-2.004384	0.511748	0.118815
6	-2.286972	-0.984562	-0.053446
6	-0.948118	-1.727647	-0.124831
8	-0.090768	-1.205797	-1.156627
8	-0.763621	2.396483	-0.798906
8	-3.227010	1.262877	0.040696
8	-2.993393	-1.546257	1.035692
1	-0.086233	2.462911	-0.102461
1	-2.980854	2.199561	-0.057019
1	0.820126	0.403160	-1.922376
1	-1.553561	0.930885	-1.941369
1	-1.553775	0.664187	1.109963
1	-2.837149	-1.131707	-0.996061
1	-0.445043	-1.677410	0.848457
1	-1.111833	-2.775088	-0.381676
1	-3.935653	-1.273430	0.979887
8	0.966964	0.472757	0.136861
6	2.942373	-0.750267	-0.654524
6	2.318248	0.175080	0.188441
6	3.052621	0.853159	1.168079
6	4.420228	0.613994	1.295992
6	5.062329	-0.296176	0.448830
6	4.317986	-0.971478	-0.519690
1	2.367395	-1.310185	-1.382895
1	2.542570	1.560321	1.816095
1	4.985924	1.144673	2.057479
1	6.128543	-0.479506	0.547937
1	4.802144	-1.690456	-1.175686
8	-5.464427	-0.260643	0.681368
1	-4.892232	0.506655	0.469274
1	-5.958579	-0.024250	1.480023

C			
6	0.280136	0.083335	-1.123084
6	-1.031455	0.869787	-1.221749
6	-2.012370	0.421298	-0.137318
6	-2.222074	-1.095771	-0.221799
6	-0.865323	-1.806577	-0.203390
8	0.006908	-1.301601	-1.225377
8	-0.764838	2.259773	-1.159226
8	-3.215617	1.163492	-0.369885
8	-2.961200	-1.612754	0.882766
1	-1.628217	2.701036	-1.086189
1	-3.819010	1.054566	0.386986
1	0.939114	0.317507	-1.964933
1	-1.466499	0.615429	-2.201127
1	-1.601083	0.673097	0.849956
1	-2.741179	-1.321299	-1.166110
1	-0.402495	-1.695549	0.785042
1	-0.986376	-2.870582	-0.416189
1	-3.846454	-1.208318	0.898796
8	0.914038	0.426519	0.093495
6	2.908495	0.963924	1.219404
6	2.266873	0.203290	0.233782
6	2.988395	-0.728808	-0.521613
6	4.361558	-0.875710	-0.292729
6	5.011111	-0.120443	0.685015
6	4.274286	0.797627	1.442904
1	2.324581	1.682712	1.786576
1	2.486481	-1.348528	-1.256170
1	4.919465	-1.599627	-0.881775
1	6.076490	-0.245719	0.858196
1	4.766660	1.394513	2.206725
8	-5.171334	0.196401	1.554386
1	-6.104670	0.300077	1.310409
1	-5.138261	0.224341	2.524003

D			
6	-0.361160	0.054213	-0.797991
6	-1.559687	0.991717	-0.547190
6	-2.548713	0.344940	0.421867
6	-2.954904	-1.034954	-0.081487
6	-1.699792	-1.877709	-0.305668
8	-0.796902	-1.219404	-1.212399
8	-1.213296	2.258080	-0.012988
8	-3.738315	1.124231	0.551648
8	-3.772720	-1.722162	0.858326
1	-0.335054	2.544571	-0.337725
1	-3.471127	2.024593	0.801744
1	0.259920	0.426639	-1.619127
1	-2.056847	1.116959	-1.521971
1	-2.065745	0.240396	1.403916
1	-3.491942	-0.918575	-1.035617
1	-1.203160	-2.075488	0.652261
1	-1.947891	-2.829932	-0.778159
1	-4.489675	-1.117378	1.112920
8	0.417113	0.011798	0.393865
6	2.567704	0.227357	1.325895
6	1.756285	-0.287672	0.303828
6	2.316839	-1.062234	-0.720344
6	3.695480	-1.298238	-0.719959
6	4.513480	-0.785470	0.289994
6	3.940984	-0.026643	1.316391
1	2.103384	0.803454	2.121901
1	1.684554	-1.493182	-1.488721
1	4.127117	-1.900451	-1.515494
1	5.581997	-0.981570	0.282992
1	4.562902	0.369999	2.115055
8	1.459344	2.833159	-0.824034
1	1.844489	3.720635	-0.882512
1	2.056196	2.311890	-0.258825

E			
6	-0.228654	-0.015922	-1.002521
6	-1.534569	0.800550	-0.943383
6	-2.487191	0.240692	0.120169
6	-2.696654	-1.253656	-0.105271
6	-1.341976	-1.959220	-0.141477
8	-0.487777	-1.386771	-1.146611
8	-1.335441	2.196188	-0.808068
8	-3.766036	0.868296	0.046366
8	-3.460584	-1.848705	0.936995
1	-0.962275	2.396116	0.079094
1	-3.622084	1.829438	0.012437
1	0.362550	0.264577	-1.878062
1	-2.010790	0.671242	-1.922137
1	-2.062071	0.390232	1.124437
1	-3.204762	-1.389964	-1.072552
1	-0.865142	-1.903231	0.844935
1	-1.457138	-3.009006	-0.417166
1	-4.270415	-1.321803	1.041342
8	0.548153	0.252348	0.183592
6	2.741053	0.845762	-0.646204
6	1.916487	-0.002893	0.097899
6	2.451790	-1.070159	0.819785
6	3.831540	-1.291637	0.793186
6	4.666621	-0.456275	0.045462
6	4.118306	0.610482	-0.673418
1	2.306237	1.681615	-1.187891
1	1.789269	-1.712932	1.391258
1	4.251653	-2.122288	1.354222
1	5.738386	-0.633709	0.024567
1	4.762806	1.267929	-1.251149
8	-0.252055	2.435687	1.794867
1	0.379953	3.120886	2.058935
1	0.273221	1.648216	1.555242

F			
6	-0.363089	-0.223114	-1.038269
6	-1.640555	0.631155	-0.992892
6	-2.466441	0.284819	0.251456
6	-2.736487	-1.216728	0.289740
6	-1.413097	-1.979214	0.210431
8	-0.664780	-1.594173	-0.958226
8	-1.403785	2.022296	-1.104956
8	-3.726523	0.953071	0.232577
8	-3.386938	-1.613077	1.491653
1	-0.727498	2.320525	-0.457037
1	-3.555449	1.886339	0.017922
1	0.162053	-0.084467	-1.988349
1	-2.227933	0.362980	-1.878497
1	-1.910017	0.569809	1.157184
1	-3.359018	-1.477880	-0.580311
1	-0.822113	-1.804352	1.117489
1	-1.587920	-3.051389	0.105303
1	-4.165480	-1.042076	1.601687
8	0.464664	0.213650	0.037940
6	2.541560	0.458435	1.104902
6	1.800455	-0.121497	0.064419
6	2.424991	-0.970860	-0.856725
6	3.800256	-1.203279	-0.744520
6	4.551153	-0.613994	0.274587
6	3.911239	0.212371	1.204370
1	2.026011	1.069925	1.841513
1	1.853485	-1.469605	-1.630597
1	4.281166	-1.864203	-1.461202
1	5.617387	-0.806435	0.352682
1	4.476553	0.663432	2.015937
8	0.620624	3.306098	0.411108
1	0.840087	4.129295	-0.051731
1	1.412676	2.746623	0.352222

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm ⁻¹	Intensity / km mol ⁻¹	Frequency / cm ⁻¹	Intensity / km mol ⁻¹	Frequency / cm ⁻¹	Intensity / km mol ⁻¹
v1	30.5158	0.5425	26.4454	1.4000	12.7281	9.1009
v2	41.5590	0.9538	34.8439	2.9181	34.1592	1.5885
v3	46.4177	0.2374	45.7016	0.2514	48.6097	0.8058
v4	65.3192	1.0822	74.5843	0.5135	67.7609	0.7725
v5	104.1764	0.4716	97.5069	2.7755	91.4634	7.6068
v6	135.9749	1.6548	132.9498	1.8258	102.6044	0.3469
v7	143.2050	12.1158	149.6932	6.1065	121.3321	4.4763
v8	159.8021	2.3252	176.7920	2.7569	134.4892	0.8413
v9	200.0356	14.5070	188.9193	12.2715	147.7964	5.2575
v10	208.6611	70.3848	201.0530	76.7312	176.8842	3.1902
v11	228.8475	31.7239	214.5984	7.4375	193.9429	1.3950
v12	263.6686	46.2354	265.4493	19.5175	215.9476	12.6915
v13	276.5629	21.4434	268.8675	28.3007	225.9752	107.4399
v14	287.6592	19.6308	297.5839	6.1450	263.1849	2.4405
v15	333.6620	21.8436	314.1528	18.7029	288.7341	10.8227
v16	336.5062	21.8993	333.3004	11.3493	292.4812	7.5077
v17	347.6508	1.5042	357.5997	2.3064	342.3378	4.8495
v18	407.9428	3.3743	405.3549	40.6709	353.4767	16.3215
v19	421.7111	7.8086	414.7433	16.6617	396.8385	101.1483
v20	426.3130	125.3467	423.4193	0.3263	414.8677	6.3703
v21	454.6364	17.3655	445.9160	12.4987	424.9473	0.1389
v22	467.1045	45.2942	461.7704	43.4579	442.8410	6.4394
v23	505.3693	0.0689	503.5425	61.2483	497.0418	7.8668
v24	518.7928	7.7771	506.8562	135.4900	518.2231	11.1880
v25	533.4024	31.0472	518.3095	27.8101	531.5352	8.4449
v26	543.1119	16.3088	538.7187	38.2228	537.0325	214.7705
v27	562.7951	80.4613	544.3666	4.1641	550.4141	9.1868
v28	578.1240	11.8035	579.9350	27.1758	572.6147	41.7175
v29	625.3773	0.2893	625.3151	0.4972	588.2111	15.5005
v30	653.3552	13.0603	652.9090	14.6760	625.7485	0.9253
v31	698.8836	19.1401	699.4659	20.6743	652.8609	20.5554
v32	733.0429	10.2352	732.8997	8.5201	700.6877	22.5591
v33	762.9454	123.2654	742.4131	129.7999	733.3899	16.5764
v34	765.8694	56.0315	766.0159	69.6738	765.4695	64.5663
v35	837.8579	0.0880	837.8165	0.0984	842.3379	0.3405
v36	859.9695	38.9751	861.4933	53.0884	861.4346	34.6422
v37	907.4202	13.6911	904.0636	0.6721	909.1673	15.3494
v38	914.4015	1.1150	908.4424	13.5580	910.3337	5.0661
v39	923.6218	47.5236	926.3651	33.7791	934.3179	18.0986
v40	955.5693	40.1795	956.2198	37.2229	952.0639	55.2316
v41	972.1798	0.3970	972.3662	0.3382	972.6711	0.3721
v42	993.7312	0.0952	993.5057	0.1086	990.2757	0.1330
v43	1009.6657	94.9571	1009.0804	135.4329	1013.8884	5.2499
v44	1018.2422	54.1249	1018.2298	73.8220	1028.0810	154.9338
v45	1049.7901	238.6700	1052.2855	61.3401	1046.4045	83.5965
v46	1052.0550	35.9333	1053.2566	72.9964	1052.9078	16.9945
v47	1060.2555	122.6025	1071.2802	190.3625	1065.6177	308.3415
v48	1102.5024	34.6296	1099.6190	93.3600	1101.5535	46.8754
v49	1110.7698	13.2424	1109.1011	11.5700	1108.5995	14.8868
v50	1116.2002	95.8717	1111.9753	79.5166	1113.9823	133.0688
v51	1139.7317	52.1610	1129.6522	25.5795	1124.1669	54.1375
v52	1144.1195	107.3224	1147.1343	111.6438	1149.8629	34.6254
v53	1155.8310	33.4283	1159.3326	28.2075	1154.0597	11.0244
v54	1188.4631	3.0815	1188.2705	2.6945	1186.5109	2.4845
v55	1205.9330	15.5227	1204.5301	17.3130	1204.9972	12.6617
v56	1220.6330	60.7612	1219.5941	34.5858	1222.7551	69.7777
v57	1233.1990	17.9602	1231.9737	17.4939	1233.7700	56.4284
v58	1246.2867	253.6515	1249.1147	292.0238	1253.3228	114.6962
v59	1258.3607	51.7585	1260.8602	23.7145	1267.0130	190.2934
v60	1283.2962	43.2175	1287.4114	72.6803	1271.5875	21.9295
v61	1303.0935	14.0888	1315.6467	5.8140	1293.9392	14.7560
v62	1310.6780	9.9763	1328.0201	10.5355	1321.7299	12.6870
v63	1345.2606	1.1708	1344.8651	3.2142	1342.8787	4.3788
v64	1359.8144	9.6903	1359.7054	57.9038	1362.5512	5.1483
v65	1367.6601	3.4840	1365.7527	8.6086	1368.7804	5.2165
v66	1381.4531	57.1353	1371.8559	16.4674	1385.6733	32.6132
v67	1400.0530	4.8495	1393.5252	23.0089	1399.5964	2.7149
v68	1406.9623	30.9944	1407.4179	8.5675	1401.9261	12.6965
v69	1411.1092	25.2337	1414.4037	8.6605	1412.2343	70.6763
v70	1442.5138	26.8495	1440.3964	13.9197	1438.3137	8.4678
v71	1448.5366	18.9562	1441.8389	30.3214	1446.6570	9.2492
v72	1471.0338	22.7498	1484.5061	17.0875	1453.6852	11.0891
v73	1498.6562	0.7703	1498.2823	0.6342	1497.8322	0.5508
v74	1526.3580	3.5843	1524.4137	3.3153	1527.1476	3.4945
v75	1536.3642	98.1972	1535.8725	101.4041	1537.2147	104.9156

v76	1640.1547	25.2773	1639.3753	24.1948	1637.4835	22.1001
v77	1652.1756	62.2763	1651.9355	63.1693	1652.4640	75.1156
v78	2577.1489	184.0226	2597.9942	153.6748	2689.6837	22.9284
v79	2791.1938	98.9868	2793.6177	95.7721	2820.8586	56.9967
v80	3002.4708	12.4021	3011.6153	16.3898	3004.9188	6.4199
v81	3019.1956	40.9333	3038.2852	25.8085	3014.0348	41.1840
v82	3069.5647	33.0453	3069.7288	32.1342	3049.8008	30.4345
v83	3090.9526	15.7169	3091.6468	12.7182	3065.8647	42.8818
v84	3109.1146	21.1024	3101.5450	27.4213	3099.1024	22.8459
v85	3150.9270	17.4987	3156.7515	15.7575	3143.2270	21.2395
v86	3185.1537	1.6100	3184.8104	1.4255	3180.4831	0.9830
v87	3192.7096	10.1980	3192.7017	11.1364	3188.9344	18.4160
v88	3204.0098	23.6283	3204.5548	25.4716	3204.2844	32.3521
v89	3212.4945	14.9663	3212.4121	13.9659	3213.6582	7.8200
v90	3235.2329	0.7317	3233.7304	0.6291	3230.9841	1.1429
v91	3516.6823	601.8538	3522.8405	644.3528	3677.0345	107.0086
v92	3688.7790	87.0837	3703.6386	57.1803	3702.0323	412.5644
v93	3715.9116	51.3559	3708.8368	50.3918	3721.6795	54.5166

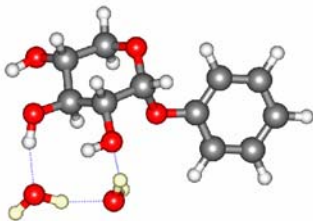
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	30.8191	2.7764	13.4413	0.7081	24.8997	1.3964
v2	40.1348	4.3273	32.7276	1.4712	36.5888	0.9746
v3	49.4082	0.0176	39.2092	5.0769	47.3989	1.7802
v4	61.3017	1.5379	52.7049	3.6281	72.2491	1.2120
v5	74.2294	6.2461	56.4491	3.1449	85.3573	2.5176
v6	107.1720	1.4721	117.2810	0.6529	102.2506	8.9510
v7	129.2840	52.2508	122.8341	58.1713	114.0396	11.1467
v8	133.4557	1.3427	128.4896	35.4294	143.8891	41.8927
v9	137.4755	4.3166	140.7718	11.3110	161.1047	3.6724
v10	190.9840	35.6159	162.8024	4.4748	190.7270	16.1886
v11	196.6089	3.2672	192.1045	0.8632	204.6856	9.1907
v12	213.2776	8.3601	210.2619	1.8134	235.3487	12.6431
v13	238.4871	53.6332	226.1265	1.8046	252.1643	68.9618
v14	241.0383	18.0241	251.5473	35.4451	258.8086	63.4086
v15	269.3933	3.6198	269.5387	30.1123	279.5544	17.0427
v16	299.6483	12.8362	275.5898	9.7548	291.3525	9.0600
v17	333.5125	9.8377	284.5109	1.1822	337.8133	15.7738
v18	344.8839	6.7790	299.2237	2.6372	355.6245	4.8933
v19	387.0413	92.2849	354.5878	13.8409	384.6702	110.7990
v20	406.1400	109.4443	368.8632	4.8859	403.9160	62.9641
v21	420.7213	27.3272	388.9579	1.2555	415.8306	10.3682
v22	424.5735	0.0903	411.3677	83.8240	424.1009	0.0943
v23	442.9341	8.6568	423.7801	1.0281	439.6936	3.8445
v24	499.9168	12.6532	429.7167	6.1224	499.7343	7.4973
v25	519.3555	17.1924	441.3517	7.4253	518.2017	14.5627
v26	530.1675	16.1764	502.4613	39.8379	531.6776	4.1798
v27	548.0458	19.5148	518.3674	15.5964	550.7124	2.5808
v28	575.6410	4.9953	535.0395	15.2598	579.9068	17.7892
v29	605.3139	116.0692	554.0391	8.8064	625.8893	0.7621
v30	625.1601	7.1357	563.9917	224.5768	657.6120	16.6750
v31	647.0819	8.5667	626.6944	0.5918	701.3928	17.3257
v32	701.9061	17.7360	650.0590	3.6685	729.4700	14.2613
v33	735.2864	15.5171	687.9802	29.9667	744.3483	139.3919
v34	767.6628	68.8296	703.8567	18.6750	764.5069	82.5760
v35	847.4817	0.3720	708.5250	35.4670	838.1292	1.4288
v36	863.0554	34.0904	753.4316	8.1990	859.8945	41.2901
v37	910.5884	3.7186	766.6606	54.3586	904.2569	8.3700
v38	912.1881	15.2234	800.2217	20.1294	909.9588	0.6736
v39	932.7229	24.1717	839.6496	0.3645	932.4588	39.8851
v40	950.1657	49.2964	856.2036	66.5015	950.7557	42.1542
v41	977.5655	0.6053	884.1425	7.7237	972.5559	0.9397
v42	995.1498	0.2576	908.6801	5.4524	993.1155	0.2354
v43	1012.6580	17.2764	928.2121	9.4230	1010.7818	56.5383
v44	1023.6576	241.0801	971.9587	0.2127	1018.4759	168.1073
v45	1046.9493	61.4412	983.6676	76.8914	1045.0528	93.2185
v46	1051.4510	28.5495	991.8989	1.3511	1053.0473	19.2013
v47	1070.4324	219.8991	1013.4986	16.2230	1068.3556	162.9702
v48	1101.4189	77.7702	1015.2611	10.6173	1106.7643	117.2380
v49	1106.0474	12.0511	1034.5639	365.2622	1110.8957	12.5930
v50	1119.8165	121.6621	1036.2668	28.9360	1122.8752	109.3571
v51	1134.4428	20.7407	1052.4957	56.3930	1131.9661	30.4123
v52	1142.7922	87.1309	1094.0983	113.6785	1153.7679	30.9458
v53	1153.9521	34.1317	1101.1437	148.5518	1158.3661	57.9406
v54	1187.3583	2.2740	1109.8735	7.3272	1188.3722	2.8670
v55	1202.1679	14.2032	1116.7477	58.0785	1206.9269	26.6569
v56	1223.6742	26.1212	1128.4547	19.7539	1224.5309	4.5811
v57	1227.5699	53.8394	1171.0008	28.7494	1225.8863	67.9953
v58	1256.3852	19.5598	1184.1014	23.0069	1253.4400	53.3057
v59	1263.7831	263.5214	1187.3482	4.7803	1259.6025	250.5053
v60	1281.7326	12.9039	1205.3941	16.3205	1294.0542	15.6754
v61	1301.6012	24.6332	1233.0406	41.9275	1308.7774	36.9100
v62	1337.0165	1.2129	1233.3219	21.6674	1321.4038	25.0132
v63	1351.7228	17.2536	1242.8613	88.5675	1346.9827	8.2522
v64	1360.8984	30.1325	1261.2147	260.3767	1359.5710	42.8833
v65	1365.9328	20.9462	1286.5926	52.7102	1364.0214	8.8804
v66	1367.1811	0.3809	1301.4265	2.0407	1369.5471	4.4551
v67	1388.9194	38.8405	1329.7708	10.7766	1389.2582	20.2931
v68	1396.5684	6.6677	1344.1459	6.5467	1399.2312	35.2324
v69	1413.8914	30.0956	1366.9238	2.5001	1416.5451	3.8329
v70	1436.6843	13.2126	1375.2738	7.4397	1440.9312	13.0663
v71	1449.3476	2.3013	1380.6573	3.5623	1448.4370	6.5795
v72	1470.3660	9.6173	1404.5389	22.3811	1453.3161	47.2202
v73	1496.3081	0.8960	1412.3871	54.8591	1497.7363	0.5681
v74	1525.3075	3.5414	1426.8020	17.2123	1527.6560	4.0399
v75	1534.9196	99.9167	1427.1186	28.6394	1536.3270	99.3477

v76	1635.0135	16.8248	1437.8209	2.9174	1637.6213	22.6427
v77	1649.1856	75.1350	1441.8174	15.5746	1650.5977	76.3736
v78	2670.6074	34.8579	1442.8272	34.7420	2682.9975	23.2526
v79	2811.8752	92.8159	1498.0150	0.6418	2816.2247	86.9819
v80	3005.7427	7.7800	1509.9324	7.8811	3009.0485	13.3877
v81	3013.2589	34.1190	1517.8635	4.7258	3027.0237	33.7609
v82	3041.2278	41.8961	1536.6910	97.5850	3070.0852	29.9396
v83	3065.9235	42.4362	1638.9011	22.5603	3080.8716	31.2820
v84	3092.4248	18.4763	1652.2634	66.1506	3098.4442	28.2801
v85	3147.2469	19.8268	2610.5068	146.6713	3149.6914	18.6559
v86	3183.9622	1.5876	2794.5478	77.3333	3183.6162	3.4661
v87	3191.6980	12.0181	3019.5384	28.1299	3190.6397	5.4941
v88	3203.4296	16.8955	3052.2823	10.3845	3199.4276	18.4371
v89	3211.3958	15.7928	3062.5367	16.5404	3211.7097	19.9041
v90	3230.5090	0.4639	3085.1997	20.9798	3234.7050	1.7653
v91	3587.0658	447.7917	3101.0603	19.4994	3537.3390	432.0685
v92	3730.8832	44.1481	3115.3184	5.2755	3716.4331	46.6511
v93	3735.4627	52.8324	3130.3572	19.7090	3734.2653	49.0041

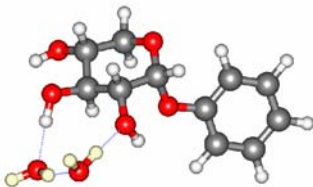
Table 12. α -PhXyl•(D₂O)₂

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

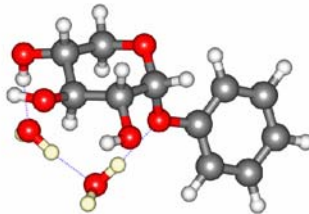
Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6- 31+G(d) energy / kJ mol ⁻¹
A	4.20	0.00
B	0.00	2.25
C	14.61	4.52



A



B



C

(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	-0.150754	-0.744177	0.981500
6	1.258710	-0.201436	1.254642
6	2.170014	-0.386089	0.034460
6	2.169976	-1.860051	-0.370216
6	0.732482	-2.318172	-0.610886
8	-0.075308	-2.085947	0.556714
8	1.158907	1.167946	1.658825
8	3.503329	0.011984	0.330512
8	2.906151	-2.068779	-1.566691
1	2.046704	1.453136	1.936109
1	3.637001	0.932216	0.008722
1	-0.751175	-0.760530	1.896433
1	1.667665	-0.790807	2.086165
1	1.781581	0.202420	-0.807336
1	2.606786	-2.450299	0.450922
1	0.309737	-1.797827	-1.479366
1	0.686919	-3.394238	-0.788626
1	3.773395	-1.648050	-1.435995
8	-0.771316	0.112277	0.029968
6	-4.335562	-0.905643	0.116528
6	-2.945589	-1.001584	0.247278
6	-2.154607	0.112887	-0.054079
6	-2.745664	1.304338	-0.489801
6	-4.131582	1.380456	-0.626527
6	-4.935066	0.276437	-0.321982
1	-4.948131	-1.772530	0.351283
1	-2.485114	-1.932748	0.556829
1	-2.117636	2.166061	-0.695461
1	-4.584010	2.310420	-0.961211
1	-6.014802	0.338716	-0.425343
8	0.737732	2.964617	-0.473760
1	0.267214	2.524016	-1.197539
1	0.650724	2.346235	0.287829
8	3.459051	2.670743	-0.430726
1	4.014123	3.220260	-1.001909
1	2.516509	2.929032	-0.585740

B			
6	-0.350110	0.443187	-1.010037
6	1.131734	0.018757	-0.975321
6	1.887501	0.719637	0.165837
6	1.629308	2.228092	0.091398
6	0.131515	2.512259	0.098682
8	-0.505052	1.835879	-1.001688
8	1.217703	-1.409393	-0.911920
8	3.290919	0.535789	0.079233
8	2.216189	2.899873	1.195452
1	0.608936	-1.702498	-0.210171
1	3.559713	-0.272555	0.575116
1	-0.836260	0.094367	-1.926929
1	1.592098	0.301131	-1.926667
1	1.513335	0.349273	1.131812
1	2.060077	2.603314	-0.851123
1	-0.315544	2.200633	1.050474
1	-0.069174	3.574028	-0.055392
1	3.126859	2.563121	1.264204
8	-0.953302	-0.197711	0.115478
6	-4.593757	0.132438	-0.504820
6	-3.221251	0.379801	-0.625511
6	-2.327662	-0.358961	0.156816
6	-2.798612	-1.315061	1.064063
6	-4.169317	-1.542041	1.179510
6	-5.075170	-0.823178	0.391357
1	-5.287523	0.706855	-1.113483
1	-2.861631	1.153388	-1.293877
1	-2.084259	-1.868205	1.667319
1	-4.529328	-2.286664	1.884774
1	-6.142867	-1.002975	0.480623
8	3.357210	-3.190549	-0.907733
1	3.913738	-3.167968	-1.700066
1	2.621573	-2.556211	-1.067575
8	3.986226	-1.809416	1.368467
1	3.932912	-2.449203	0.617409
1	4.853124	-1.925190	1.783406

C			
6	-0.042305	-1.273400	0.382713
6	1.230427	-1.156648	1.233057
6	2.307391	-0.325801	0.541827
6	2.541048	-0.787443	-0.899170
6	1.198698	-0.885482	-1.634883
8	0.274379	-1.721991	-0.911516
8	0.892883	-0.629126	2.510435
8	3.486919	-0.440348	1.339838
8	3.459092	0.070640	-1.560508
1	1.715232	-0.598516	3.027702
1	4.214177	-0.029278	0.841519
1	-0.712238	-2.027529	0.804665
1	1.610611	-2.183853	1.338249
1	1.987506	0.723398	0.523884
1	3.014105	-1.776171	-0.880769
1	0.764375	0.110821	-1.786897
1	1.325937	-1.363539	-2.607975
1	3.082522	0.979394	-1.579436
8	-0.729692	-0.017957	0.373301
6	-4.087988	-0.923623	-0.915999
6	-2.708853	-0.999350	-0.692073
6	-2.094251	-0.024256	0.100567
6	-2.842157	1.023386	0.647931
6	-4.213769	1.092069	0.403182
6	-4.845490	0.116911	-0.375683
1	-4.564535	-1.683222	-1.530482
1	-2.121519	-1.789737	-1.144923
1	-2.348713	1.770839	1.261304
1	-4.790389	1.907629	0.831859
1	-5.914805	0.170548	-0.560324
8	2.237979	2.637131	-1.335014
1	1.551043	2.757348	-0.637184
1	2.051184	3.285216	-2.029366
8	0.352867	2.619856	0.715791
1	-0.020615	1.713263	0.710872
1	0.704205	2.749576	1.609865

(c) Vibrational frequencies.

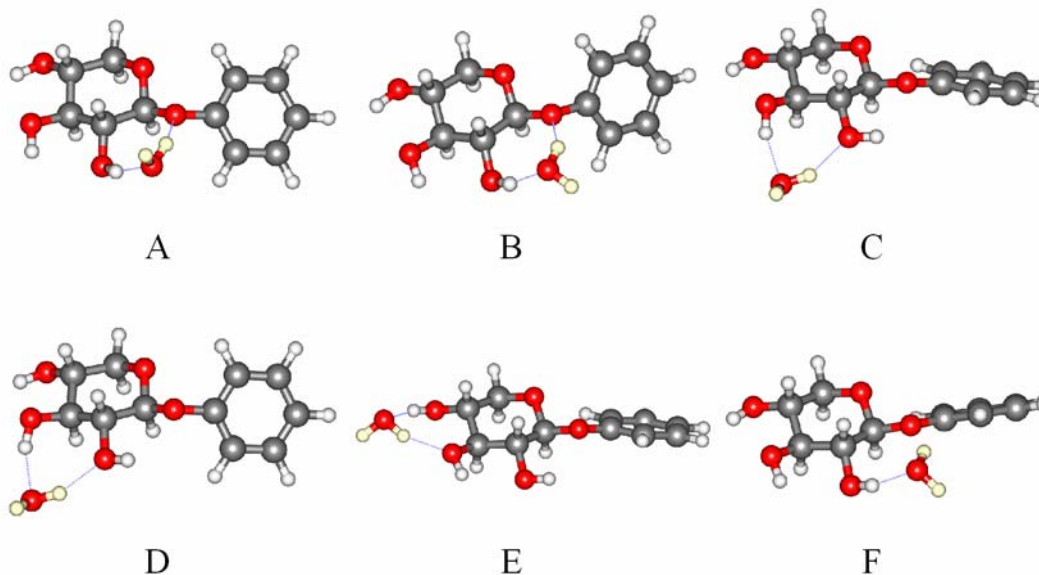
	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	22.0442	3.8113	23.8662	0.8504	18.6298	0.8089
v2	26.8017	0.8579	30.7972	4.0909	37.4772	0.2085
v3	46.1031	0.2280	36.5932	0.6413	47.7537	1.5993
v4	52.2379	0.4019	41.5875	1.7257	53.4343	0.8608
v5	60.0906	2.3625	51.6615	0.8938	76.8184	0.0228
v6	80.6827	7.1605	78.9858	4.4557	87.9674	29.6599
v7	104.4973	23.9714	106.8334	2.9066	98.3472	18.8413
v8	121.5655	16.8976	134.9729	12.6031	114.1484	3.0779
v9	125.9211	9.2751	148.8707	5.7024	119.4414	18.7097
v10	171.2939	1.5559	172.1821	20.5853	154.5249	4.5441
v11	191.2381	33.4984	184.1237	19.9605	180.0490	3.7111
v12	210.7132	3.2712	194.8787	41.9661	194.8639	1.5326
v13	219.2749	1.8594	207.1517	8.9119	214.0995	28.5164
v14	239.2835	30.9416	223.0373	4.5976	220.9477	74.5584
v15	242.3861	20.0858	248.8607	9.3520	240.3197	7.7964
v16	261.0444	16.0628	262.2999	11.6776	243.5805	19.2674
v17	266.9610	7.7921	270.8866	34.8092	251.8620	37.8883
v18	276.7805	37.5240	293.3436	25.2442	259.4336	15.9508
v19	287.8841	34.7729	301.3178	43.5496	289.7451	7.6502
v20	337.9521	3.4209	341.3890	13.6752	338.0053	4.1675
v21	351.8217	24.3711	352.7267	11.7253	343.3129	8.8299
v22	380.3225	98.1515	385.5968	131.3801	359.0667	24.1759
v23	406.6039	56.3372	410.6619	4.6402	399.2231	101.8647
v24	417.2069	33.9244	422.7429	0.6835	405.0264	61.3510
v25	425.8540	0.5537	433.5173	94.4910	419.9178	18.7848
v26	443.8800	51.3561	459.4019	56.0532	422.7980	4.2778
v27	462.0858	121.4986	471.0781	66.7347	440.2348	2.3343
v28	496.6213	4.3473	500.2546	5.7351	496.2660	55.0281
v29	519.3041	10.4753	517.5183	14.7110	508.1486	52.4246
v30	532.5459	5.9018	523.9534	23.6661	517.5822	11.1927
v31	558.6504	1.3487	536.7379	27.2169	533.5395	2.1588
v32	578.1811	19.7186	545.1442	22.4035	555.8131	3.2152
v33	585.5712	77.9280	570.0952	49.2514	578.4146	11.3418
v34	598.3981	57.8962	580.6898	35.6693	606.6748	66.1770
v35	625.4462	3.1747	625.3995	0.3282	625.8380	2.7883
v36	650.3434	15.5909	653.3616	17.0986	651.1994	24.3562
v37	707.0074	27.5589	699.0377	19.7148	700.7395	23.8964
v38	731.2764	11.0136	733.9785	11.7525	733.6327	8.5560
v39	769.8670	79.6555	765.6362	71.4244	748.8588	124.6853
v40	771.0989	15.4735	838.1299	1.4310	767.0644	67.4219
v41	842.5237	0.4226	843.1974	66.7207	842.0538	0.1253
v42	858.8486	42.1509	860.1360	36.1404	863.6327	57.5544
v43	912.9734	16.0101	908.4453	13.6360	907.7242	53.1238
v44	914.6967	2.3904	915.8636	1.4268	910.2515	1.8657
v45	928.7625	12.3293	925.4989	51.9749	923.1048	13.2288
v46	947.1036	49.5318	953.8931	38.3460	944.6582	49.5438
v47	975.4081	0.7005	972.1409	0.4671	975.9113	0.8341
v48	995.6630	0.2049	992.7878	0.1245	995.3261	0.7670
v49	1013.1519	64.4755	1011.0292	72.2782	1005.8370	156.8374
v50	1021.7152	168.8282	1019.2953	82.4751	1017.7270	24.2905
v51	1044.6524	73.4089	1052.2194	19.6481	1054.8244	15.5835
v52	1053.0853	20.3921	1052.6027	187.7995	1061.0790	288.8458
v53	1065.1414	275.5837	1063.7407	192.9677	1072.2946	99.3855
v54	1108.5332	20.8535	1104.9595	42.3863	1110.1202	135.2757
v55	1110.7857	12.0843	1109.5729	9.5829	1112.7563	12.2856
v56	1120.4658	71.9753	1119.8945	98.2840	1116.1724	27.3818
v57	1138.5198	71.9145	1139.8490	73.2420	1134.4822	46.9544
v58	1144.2202	68.8698	1144.2318	91.6118	1145.2413	41.7632
v59	1152.1894	8.5262	1155.6943	31.4626	1155.6408	4.3661
v60	1188.9244	1.0460	1188.2413	2.5675	1190.4534	1.3537
v61	1204.3663	11.8178	1204.7262	16.3788	1209.6014	16.7513
v62	1232.0856	32.0198	1227.5027	30.4739	1233.6015	114.4260
v63	1237.8346	67.6736	1240.2179	34.5869	1238.5691	64.4144
v64	1242.2352	134.0727	1246.4855	271.0356	1241.6156	95.3513
v65	1248.9594	175.0833	1255.1645	31.1661	1249.3229	40.8462
v66	1271.2195	27.4421	1261.8584	49.7831	1264.0322	34.2703
v67	1275.8921	29.0282	1286.0720	34.0379	1266.6512	6.6189
v68	1299.6874	9.3547	1302.3978	11.8860	1297.2662	24.2965
v69	1331.9350	3.1374	1311.1851	11.3392	1342.6335	8.0287
v70	1343.8029	0.1685	1345.3894	1.1631	1343.5773	7.8543
v71	1359.4821	5.9456	1360.8645	6.9630	1358.9801	27.3589
v72	1366.3146	5.4919	1367.3778	6.3801	1370.0370	2.5229
v73	1387.5773	28.2952	1382.8878	54.2736	1376.7080	3.3225
v74	1401.7196	17.1881	1402.3728	10.1452	1401.5055	22.3929
v75	1410.0455	52.5292	1404.5085	0.9420	1407.3034	17.4991

v76	1423.0553	26.9728	1413.8866	45.7092	1425.5310	2.1899
v77	1433.5285	2.1218	1446.2649	16.3348	1442.5243	20.0731
v78	1445.6974	5.9085	1449.2074	28.6583	1452.2690	8.9627
v79	1477.9139	15.6831	1468.9430	15.3132	1482.3340	55.2490
v80	1497.3381	0.6235	1498.1837	0.6095	1498.8824	0.6763
v81	1526.9259	3.0770	1531.0923	5.9922	1526.7988	4.3991
v82	1536.1001	100.9318	1536.0033	98.6151	1537.1982	97.9153
v83	1638.5180	19.6086	1639.2428	24.6662	1640.4370	21.1931
v84	1651.3192	63.0789	1651.8993	64.4018	1651.3287	59.4892
v85	2473.7862	304.2576	2492.8016	229.8989	2515.4747	297.8269
v86	2557.7674	205.7339	2558.3769	404.7629	2601.3614	164.1213
v87	2777.1440	42.0291	2785.8140	94.4919	2782.7130	91.9183
v88	2793.7588	76.6135	2789.2685	67.1610	2791.0075	67.2771
v89	3005.8581	23.6438	2998.7058	25.6727	3023.7966	17.9618
v90	3044.7760	3.5772	3031.1217	24.6583	3059.6684	11.9707
v91	3058.3635	20.1090	3069.3026	33.3165	3063.8475	2.3160
v92	3066.1320	58.7259	3091.8727	16.5034	3082.7033	59.5797
v93	3098.0603	21.6865	3110.0883	21.9247	3109.5478	18.4882
v94	3146.8639	19.4175	3148.5475	19.0774	3146.4253	20.0615
v95	3184.0989	1.0829	3184.5979	1.3647	3185.2770	0.5199
v96	3192.3143	13.2691	3192.4521	11.6378	3194.0356	15.6274
v97	3205.8328	27.9992	3204.5205	25.0925	3208.0462	27.0355
v98	3213.4976	9.4465	3212.3379	13.3939	3217.8316	4.6856
v99	3233.8827	0.5171	3234.4383	0.6709	3235.3994	0.4963
v100	3498.4671	659.1480	3462.8038	891.7628	3518.6485	363.5008
v101	3716.7013	34.6339	3702.2702	71.0762	3719.9768	51.9514
v102	3722.0544	65.0864	3708.0251	46.5698	3730.2891	51.2787

Table 13. β -PhXyl $\cdot$ D₂O

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	4.73	0.00
B	5.22	0.56
C	0.00	3.58
D	3.88	4.74
E	0.11	4.77
F	7.30	7.19



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.281823	-0.075671	-0.057125
6	1.484348	0.874319	0.066993
6	2.732617	0.160623	-0.458938
6	2.934760	-1.184172	0.230162
6	1.652184	-2.009032	0.107679
8	0.542114	-1.282322	0.642511
8	1.345659	2.060582	-0.695988
8	3.904499	0.941835	-0.248917
8	3.989258	-1.928781	-0.366300
1	0.775295	2.688656	-0.202482
1	3.731124	1.822105	-0.624589
1	1.622053	1.105336	1.133835
1	2.598835	-0.017336	-1.538776
1	3.148882	-1.006480	1.295067
1	1.473591	-2.271350	-0.946636
1	1.722821	-2.931081	0.687825
1	4.768455	-1.349307	-0.407100
8	-0.851188	0.530886	0.533116
1	0.065062	-0.293427	-1.115702
6	-4.636546	-0.923356	-0.490490
6	-3.837758	-1.638974	0.407127
6	-2.564753	-1.174297	0.749192
6	-2.100268	0.009917	0.173690
6	-2.885444	0.736513	-0.722479
6	-4.159588	0.264829	-1.051605
1	-5.626955	-1.288556	-0.748725
1	-4.206425	-2.561416	0.848376
1	-1.931560	-1.712379	1.445642
1	-2.498488	1.658338	-1.147588
1	-4.776804	0.827503	-1.747055
8	-0.552781	3.303871	0.941546
1	-0.869089	2.388063	1.073694
1	-0.425536	3.688575	1.821236

B			
6	-0.277756	-0.055622	0.081352
6	-1.500356	0.863127	-0.065656
6	-2.736825	0.116545	0.440630
6	-2.889405	-1.233323	-0.252043
6	-1.588209	-2.025445	-0.106298
8	-0.486407	-1.270199	-0.617673
8	-1.397478	2.051896	0.702272
8	-3.926822	0.863640	0.211503
8	-3.934590	-2.006482	0.324681
1	-0.861264	2.701007	0.197444
1	-3.779021	1.754636	0.572501
1	-1.625345	1.095303	-1.133054
1	-2.615953	-0.058074	1.522748
1	-3.088403	-1.060324	-1.320524
1	-1.423705	-2.285923	0.950898
1	-1.623824	-2.947540	-0.689473
1	-4.731516	-1.450527	0.344293
8	0.849217	0.578820	-0.492613
1	-0.075869	-0.263784	1.145202
6	4.637012	-0.903500	0.472107
6	3.987169	-1.341222	-0.686550
6	2.711924	-0.866173	-1.004378
6	2.098574	0.051150	-0.151182
6	2.734769	0.499887	1.007569
6	4.009291	0.015974	1.317763
1	5.628535	-1.276536	0.714175
1	4.472020	-2.056971	-1.345297
1	2.185602	-1.197161	-1.893483
1	2.233775	1.218541	1.650732
1	4.510861	0.361412	2.218014
8	0.372386	3.320562	-1.050054
1	0.819730	2.450916	-1.046559
1	1.046784	3.980745	-0.832411

C			
6	0.022860	-0.193017	-0.091878
6	-1.238090	0.596234	-0.472303
6	-2.478830	-0.099408	0.096744
6	-2.475726	-1.574437	-0.320668
6	-1.148415	-2.237539	0.043730
8	-0.058441	-1.526048	-0.554206
8	-1.150890	1.927085	0.057850
8	-3.700973	0.447339	-0.371463
8	-3.516757	-2.286882	0.329148
1	-0.317686	2.312938	-0.261226
1	-3.876638	1.294399	0.095774
1	-1.306725	0.634498	-1.567398
1	-2.437248	-0.047583	1.196948
1	-2.607261	-1.620115	-1.412807
1	-1.032730	-2.275901	1.138448
1	-1.099344	-3.255320	-0.347447
1	-4.330225	-1.768165	0.202614
8	1.099041	0.454461	-0.719354
1	0.166507	-0.181126	1.002759
6	5.057043	-0.026415	0.529099
6	4.103366	-0.964144	0.928435
6	2.767571	-0.846957	0.527870
6	2.391405	0.236681	-0.270760
6	3.339106	1.179124	-0.684333
6	4.668036	1.043329	-0.284948
1	6.092429	-0.129939	0.841290
1	4.395348	-1.807686	1.548799
1	2.044809	-1.605270	0.804681
1	3.021946	2.004564	-1.315317
1	5.400463	1.778339	-0.608686
8	-3.610779	2.911388	0.942963
1	-2.665264	2.876672	0.688050
1	-3.987945	3.690253	0.508084

D			
6	0.040817	-0.121295	-0.092673
6	-1.277119	0.486564	-0.588166
6	-2.451653	-0.173255	0.141414
6	-2.341166	-1.697877	0.015193
6	-0.959252	-2.182076	0.454235
8	0.057599	-1.518040	-0.304201
8	-1.282527	1.899779	-0.334446
8	-3.721152	0.180961	-0.383985
8	-3.313771	-2.343731	0.822062
1	-0.490457	2.269629	-0.760068
1	-3.951604	1.089625	-0.088112
1	-1.362248	0.302010	-1.667176
1	-2.396260	0.093872	1.209446
1	-2.489072	-1.962269	-1.043397
1	-0.818333	-2.002919	1.531498
1	-0.839223	-3.249545	0.260379
1	-4.165749	-1.916641	0.625688
8	1.072327	0.476444	-0.840416
1	0.185662	0.092741	0.980657
6	4.999923	0.099376	0.540339
6	4.491974	-0.812585	-0.390558
6	3.173336	-0.704015	-0.839910
6	2.370457	0.326189	-0.349475
6	2.864921	1.246084	0.576824
6	4.184467	1.127164	1.022956
1	6.026404	0.010925	0.885875
1	5.122624	-1.613010	-0.768771
1	2.757630	-1.403176	-1.557874
1	2.222837	2.046024	0.936111
1	4.574633	1.841957	1.742892
8	-3.795532	2.866326	0.395674
1	-2.855091	2.839459	0.120701
1	-4.237544	3.501752	-0.186439

E			
6	0.219879	0.095630	0.052159
6	-0.946652	1.078081	-0.083843
6	-2.238168	0.438734	0.420367
6	-2.489904	-0.905628	-0.274782
6	-1.221229	-1.764215	-0.173781
8	-0.067415	-1.082815	-0.675872
8	-0.750689	2.264369	0.683895
8	-3.339677	1.329518	0.183338
8	-3.523996	-1.653439	0.334618
1	0.042261	2.714264	0.349426
1	-3.077810	2.205610	0.515135
1	-1.050451	1.324158	-1.150194
1	-2.152706	0.258262	1.502513
1	-2.713207	-0.715283	-1.335476
1	-1.067279	-2.062426	0.875448
1	-1.330118	-2.666884	-0.776683
1	-4.390861	-1.263847	0.084970
8	1.342435	0.724397	-0.504056
1	0.409916	-0.146661	1.112191
6	5.249295	-0.527756	0.285429
6	4.191807	-1.394174	0.567031
6	2.867584	-1.019796	0.312179
6	2.610340	0.248140	-0.217501
6	3.662093	1.123326	-0.509989
6	4.976636	0.731914	-0.259938
1	6.274008	-0.830991	0.481083
1	4.390509	-2.380961	0.977552
1	2.058529	-1.718222	0.490135
1	3.434682	2.098660	-0.930561
1	5.789906	1.415694	-0.489238
8	-5.710169	-0.030706	-0.343255
1	-6.432297	0.041731	0.297984
1	-5.079070	0.690755	-0.137626

F			
6	-0.311469	-0.086477	0.140669
6	-1.491304	0.896085	0.034839
6	-2.788038	0.150435	0.362832
6	-2.945201	-1.103831	-0.488775
6	-1.691928	-1.966127	-0.336007
8	-0.525974	-1.215716	-0.686091
8	-1.409271	1.967596	0.960478
8	-3.927634	0.974554	0.145157
8	-4.060793	-1.883032	-0.077143
1	-0.811162	2.657924	0.599166
1	-3.778450	1.803479	0.631665
1	-1.534528	1.268043	-0.998881
1	-2.751074	-0.151773	1.422754
1	-3.053884	-0.807444	-1.543025
1	-1.717308	-2.820879	-1.014398
1	-1.619815	-2.340439	0.697450
1	-4.833175	-1.293769	-0.048695
8	0.858505	0.554855	-0.322015
1	-0.174729	-0.395449	1.190221
6	4.693846	-1.008561	0.273513
6	4.485710	0.195114	-0.407439
6	3.193543	0.682490	-0.599770
6	2.096791	-0.034131	-0.107160
6	2.289327	-1.248632	0.557210
6	3.591967	-1.722701	0.746636
1	5.700376	-1.388762	0.422662
1	5.330531	0.758027	-0.795630
1	3.026728	1.607066	-1.146270
1	1.448001	-1.838207	0.899473
1	3.736549	-2.668232	1.262921
8	0.579826	3.430099	-0.321497
1	0.959854	2.539526	-0.449755
1	1.215344	3.922048	0.219941

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	11.8656	0.2675	23.2245	0.0358	30.6131	0.1908
v2	39.9478	0.2906	34.5504	0.4067	35.4582	2.1344
v3	51.2461	1.6688	43.7626	2.0437	53.3676	1.8670
v4	55.8126	0.2522	52.1593	1.1103	59.6579	1.6791
v5	99.2912	3.9916	99.5057	3.7717	101.9712	2.3022
v6	111.7891	2.3679	111.5165	1.3086	123.6503	3.3913
v7	139.3636	10.4610	132.4652	8.7139	140.6123	2.8301
v8	158.8741	5.8552	160.0487	7.3350	170.0657	1.3103
v9	187.5487	69.1371	177.9533	61.5990	201.8212	76.1750
v10	213.8508	6.3277	211.4367	12.0875	226.6560	3.1055
v11	228.6746	54.6389	231.6687	4.9625	236.2914	16.7930
v12	237.2413	1.9014	237.2521	15.7350	266.8155	40.3803
v13	239.1349	7.3748	261.5712	15.6445	269.4998	1.3324
v14	267.2892	5.2333	271.8554	30.5652	284.1180	9.7805
v15	298.5854	12.1334	301.8879	17.4892	295.0956	11.3271
v16	307.4297	7.0920	314.8747	20.4383	315.6300	3.6536
v17	365.1039	12.7724	382.3663	80.4145	340.1775	31.3404
v18	388.2447	111.7086	390.7525	76.2266	394.1531	60.9863
v19	408.8650	2.5655	399.3103	91.8116	414.2095	59.0254
v20	424.5587	8.1255	409.4726	0.7085	421.5563	2.5121
v21	427.4635	136.3858	424.9373	1.2095	430.8203	155.7974
v22	438.5237	2.0414	427.3054	54.1704	455.7617	51.2719
v23	457.0924	53.0817	430.4454	15.6900	467.2883	13.5145
v24	464.0814	12.0825	466.5417	2.4962	473.9897	1.4915
v25	521.0612	10.3202	518.0552	9.4393	518.6874	6.0700
v26	530.0693	19.5111	529.8289	19.2008	534.8662	18.5964
v27	540.1518	6.5729	539.5944	9.0029	539.1478	26.2502
v28	579.4945	9.6219	579.9981	8.1829	573.5654	6.2754
v29	626.9506	2.0740	628.2029	0.9508	625.0639	1.8679
v30	641.9351	17.5069	642.6025	15.9550	641.5580	11.7769
v31	660.2663	11.9871	654.7784	12.1983	670.5155	15.8613
v32	706.2532	38.1565	707.9683	41.2162	696.8524	19.0743
v33	749.6322	117.8628	730.2862	131.5243	762.1074	100.2955
v34	786.5922	47.0468	787.6331	43.1168	765.5402	77.3816
v35	840.9085	15.9196	842.6585	13.7393	835.1925	5.6390
v36	848.2489	0.6088	847.2065	0.4141	838.3614	16.5041
v37	907.4448	6.1263	907.6624	5.9575	906.0731	3.1226
v38	932.1197	5.5194	930.0198	4.6919	907.4072	7.9692
v39	980.2213	1.5517	978.1037	0.7502	970.2091	0.1637
v40	994.9036	31.5630	997.9722	19.6334	992.3906	0.1398
v41	1000.5091	1.8747	1000.1579	12.9481	1004.9175	40.5635
v42	1015.8399	94.9564	1016.1326	98.4692	1014.9065	2.9878
v43	1021.3252	76.8860	1021.4222	76.3045	1019.1997	12.0112
v44	1045.2649	9.2371	1044.6389	12.5067	1043.7191	34.8762
v45	1048.5266	146.6846	1047.6196	145.8904	1046.7322	190.0988
v46	1051.0757	28.7296	1050.3726	30.5173	1056.0871	46.2118
v47	1097.5666	211.5167	1098.9222	85.0609	1094.6714	130.5513
v48	1102.4222	35.7724	1101.8008	136.0103	1108.5183	40.9984
v49	1104.7254	70.8027	1106.2269	85.8302	1109.9472	83.2709
v50	1112.2370	45.5591	1114.4955	52.6042	1115.1867	232.8237
v51	1126.1691	143.4126	1127.5261	148.3377	1131.1589	28.6477
v52	1140.2124	16.8132	1140.3893	14.0135	1139.9883	56.4317
v53	1148.4608	28.5054	1149.6498	22.4601	1160.1974	8.2419
v54	1189.4160	0.1153	1189.1132	0.0664	1188.1840	3.0762
v55	1193.7424	18.0725	1192.0098	16.2342	1204.7702	17.8306
v56	1216.2910	55.8319	1219.2780	4.4601	1218.9703	41.9753
v57	1223.0532	91.2909	1224.8223	93.3479	1233.1497	35.6698
v58	1239.7768	95.3507	1244.3921	131.6415	1256.7116	200.1026
v59	1256.9090	27.3989	1256.7692	26.7478	1262.9862	157.6947
v60	1271.6641	23.4911	1276.0969	27.4421	1280.7547	25.0695
v61	1298.1614	28.1998	1298.7737	28.4460	1303.7530	21.3599
v62	1318.1379	11.1936	1322.4863	12.5011	1315.5460	19.5618
v63	1336.3264	2.0942	1334.6160	0.5977	1346.9261	4.5627
v64	1358.6102	0.4601	1357.7192	0.3437	1363.8868	11.0999
v65	1359.7264	10.6049	1361.2101	13.5471	1367.3855	13.3417
v66	1367.3159	23.4957	1368.3674	17.7756	1371.0965	33.9792
v67	1389.6307	34.5400	1390.2359	30.6051	1391.6105	12.3007
v68	1396.1065	45.8748	1400.7961	48.2933	1411.9000	31.6612
v69	1422.6918	14.0788	1423.9748	11.0362	1424.3425	30.3138
v70	1437.8907	23.4298	1438.5587	25.3064	1430.7106	13.6232
v71	1449.3461	4.4476	1450.0021	4.2666	1449.9530	31.4613
v72	1464.0895	11.0110	1477.1119	15.7115	1484.4496	19.0617
v73	1493.8047	1.6812	1492.7802	2.0168	1498.3874	0.5787
v74	1523.7948	4.3948	1524.1285	4.3229	1524.7662	3.5445
v75	1533.6347	68.3267	1533.1195	64.9992	1536.4620	97.0821

v76	1641.8127	7.0007	1641.9433	6.5372	1641.4156	23.7791
v77	1645.9202	34.2529	1645.5738	34.5245	1652.5277	61.5556
v78	2625.2584	112.7898	2627.1213	115.7619	2604.1926	144.1354
v79	2797.4536	106.1304	2798.6480	94.8634	2795.1246	100.6319
v80	2994.6644	3.0663	2990.9330	2.3970	2981.5608	20.9271
v81	3002.3451	17.2322	2998.8674	26.2147	3003.1081	6.3594
v82	3014.0618	1.2241	3014.1986	3.8662	3009.7446	2.4043
v83	3025.2597	25.0243	3027.3357	60.3088	3024.7484	79.7687
v84	3036.4336	106.6193	3045.1458	55.5766	3061.4530	35.6242
v85	3143.5177	19.3449	3144.2270	19.0283	3146.1633	18.4006
v86	3185.2164	0.1871	3185.0369	0.6712	3184.7595	1.4885
v87	3194.5378	12.8374	3193.5929	8.7402	3192.4630	10.8613
v88	3205.4943	23.0839	3202.9024	21.8347	3204.7891	24.4513
v89	3213.3284	8.6912	3211.2161	15.0584	3212.6274	14.7277
v90	3235.9252	1.0556	3227.8605	1.8529	3237.9924	2.1159
v91	3546.5173	504.9954	3540.3136	520.5180	3512.6840	621.2732
v92	3722.0161	48.1254	3721.8271	48.1259	3714.5082	51.1199
v93	3730.6598	49.8622	3730.9574	50.0142	3731.1303	49.2436

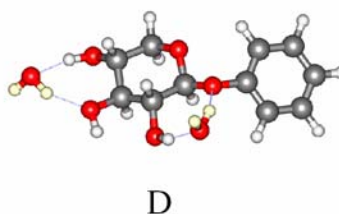
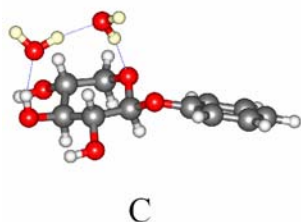
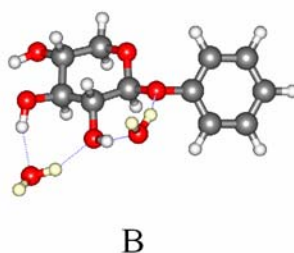
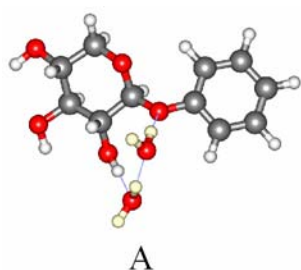
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	17.7548	0.1281	24.1593	1.4697	18.2275	0.2561
v2	30.7369	0.4868	36.0565	0.9072	45.0436	1.9654
v3	44.7018	3.4992	48.3360	0.6769	50.1267	0.4923
v4	52.9806	1.6979	60.4813	2.9768	60.2140	0.0375
v5	101.1154	2.6235	104.2636	1.8834	106.5418	6.8874
v6	111.0413	0.5463	127.6066	3.0436	117.6509	7.9018
v7	131.9721	5.4101	143.6585	6.2863	130.7997	2.2586
v8	169.4117	1.5107	171.3653	3.1340	162.9252	4.2864
v9	204.0307	76.7862	202.1081	60.2678	188.5802	42.7222
v10	218.1332	5.1120	206.0390	28.6358	214.9458	13.3337
v11	234.4216	7.3287	235.8428	0.8595	222.0678	2.2223
v12	259.3270	34.6274	266.5046	6.5971	244.4640	34.2824
v13	271.4964	12.7296	272.4696	33.7680	253.5201	17.4355
v14	282.0269	14.1756	284.0489	19.8033	275.1636	32.6511
v15	310.9369	2.8839	303.6924	4.4686	297.0003	18.6838
v16	331.1025	26.5121	316.0644	1.9464	322.3170	24.3918
v17	391.5324	35.6912	332.1046	29.8820	331.3428	1.5847
v18	395.8704	41.7120	389.0372	99.2739	386.7032	117.4935
v19	412.8050	39.6722	405.1819	19.4467	399.7073	106.3385
v20	423.9620	5.6419	420.8446	4.0483	410.6887	10.0395
v21	425.2888	41.5971	426.8843	117.6702	418.7771	0.3870
v22	443.7818	124.2570	455.5386	87.4039	433.8953	58.9282
v23	461.5863	65.9617	469.1390	10.4559	459.5654	2.7699
v24	473.6903	12.4264	471.3933	2.9501	481.9982	1.9903
v25	516.4621	5.9878	516.1334	8.3999	511.7224	5.1993
v26	534.1329	19.2799	529.9491	56.6588	532.3144	28.5880
v27	535.9847	29.9406	538.4420	11.0874	541.5745	8.8822
v28	576.0585	5.1917	576.8429	5.1855	580.7612	4.7264
v29	628.8861	0.9053	624.9603	2.7078	625.3790	2.4865
v30	638.0360	19.9098	644.5410	10.1190	642.6358	9.7294
v31	653.2426	6.4672	670.4383	22.7567	676.9829	23.3097
v32	704.1307	38.5529	694.8767	17.6523	693.6041	19.7174
v33	762.2494	105.5216	744.5350	122.5284	757.4363	110.7145
v34	784.8611	40.8374	763.8327	72.0735	762.3761	85.8817
v35	840.9018	18.0923	834.4252	2.0499	823.9763	1.5525
v36	844.2998	0.5667	838.6055	15.5572	835.8078	13.9828
v37	906.7771	6.5865	895.7457	2.7863	895.5054	2.5615
v38	925.9801	3.4974	904.2570	4.7164	909.2075	6.1643
v39	975.9723	0.2567	969.0880	0.1663	965.3177	0.4231
v40	998.1522	0.3876	990.9196	0.1163	990.8587	0.4558
v41	1004.9658	46.4722	1004.8660	33.0980	999.4995	34.8185
v42	1016.0293	17.0629	1014.7312	6.9153	1013.5311	9.9785
v43	1019.5576	3.1922	1021.7368	83.4592	1024.1132	144.0445
v44	1043.4802	29.0846	1045.2219	37.3709	1046.4843	2.6481
v45	1045.8991	216.0109	1051.5008	134.9677	1049.5899	142.8895
v46	1049.2485	21.8597	1057.1006	14.4360	1061.3528	39.8501
v47	1095.0942	126.6512	1087.8160	169.8474	1100.9451	139.1005
v48	1100.3551	4.6287	1108.7058	11.7224	1106.7973	124.2639
v49	1108.5584	284.5749	1110.7782	35.0781	1111.0834	34.2582
v50	1109.2592	77.9819	1116.4111	295.3499	1121.4018	76.7860
v51	1129.0159	35.2295	1125.8849	20.1804	1128.5984	147.7890
v52	1139.7147	38.0869	1144.7462	10.9520	1136.9220	9.1655
v53	1160.2604	6.9960	1147.2893	62.1148	1150.7159	26.2883
v54	1188.7050	0.0669	1187.8727	3.4870	1190.1154	1.3789
v55	1192.5188	16.9730	1204.3554	20.7882	1209.2097	30.3661
v56	1218.8110	43.5860	1219.5211	17.0834	1224.2733	3.5791
v57	1232.5420	58.3383	1230.3146	58.8987	1226.7705	96.6077
v58	1245.3080	164.0692	1252.6734	211.6836	1254.6064	250.4503
v59	1259.8955	58.1516	1266.0696	141.0046	1257.5612	26.3403
v60	1280.3523	20.6144	1276.4243	43.6720	1276.7535	20.0895
v61	1301.6348	19.6719	1309.0158	24.0839	1300.7581	33.3780
v62	1313.7561	19.1005	1329.0920	18.9542	1324.4547	13.4000
v63	1334.1867	0.5766	1347.0460	14.1744	1348.5923	6.5588
v64	1357.2405	0.7367	1361.0493	50.8087	1360.5724	1.4021
v65	1365.5069	9.1187	1366.5328	7.5974	1368.5750	30.3445
v66	1372.0184	40.8877	1368.9992	13.8510	1369.6953	0.3495
v67	1391.5499	11.8164	1370.4905	13.2279	1390.0678	44.9295
v68	1410.8203	32.6880	1405.4640	15.3773	1401.1125	46.0425
v69	1421.0216	22.1706	1429.5449	26.9425	1427.6746	7.3795
v70	1430.0388	10.9634	1430.5962	19.6025	1440.0678	25.2484
v71	1448.7676	33.7224	1444.2211	19.1576	1451.6130	3.1971
v72	1481.6285	15.9162	1484.5430	22.9245	1479.9170	17.4325
v73	1493.0813	1.5182	1498.5567	0.5257	1499.8492	0.6322
v74	1524.2081	3.8492	1518.9244	4.8017	1523.4783	3.8293
v75	1533.7094	65.2189	1536.1582	98.5522	1537.0936	95.5942

v76	1642.0491	5.9866	1640.6478	23.9785	1642.3605	26.7522
v77	1646.3469	37.1176	1652.6518	61.8396	1652.6185	59.1791
v78	2600.6238	152.9749	2598.2782	154.2015	2638.6270	105.3858
v79	2794.4688	100.9731	2794.1324	98.3671	2797.3694	98.4478
v80	2980.6208	19.5263	2984.8012	22.2631	2992.2119	3.7131
v81	3002.3190	6.5421	3011.4492	12.3754	3000.1935	24.3388
v82	3011.5615	4.8071	3019.1558	4.4283	3011.4402	12.4269
v83	3026.3100	78.7142	3030.1211	32.9317	3026.7721	54.8534
v84	3060.9668	34.8811	3047.7221	68.4838	3045.5185	55.8641
v85	3145.5136	19.0748	3152.6451	16.1344	3145.1133	17.9437
v86	3183.7309	1.4654	3184.3217	1.2688	3185.0383	4.1669
v87	3192.0863	7.4149	3192.2642	11.9549	3191.8895	4.4460
v88	3201.1655	25.7661	3205.1504	25.9400	3201.0691	23.9245
v89	3210.1368	17.0556	3212.6808	13.5873	3212.8132	18.8661
v90	3226.4728	2.2913	3237.3279	2.3506	3241.7378	4.6539
v91	3515.0032	613.9568	3522.2897	648.3511	3527.4602	539.6729
v92	3713.7220	50.1528	3722.5498	56.1915	3722.8469	49.1814
v93	3728.6044	52.1105	3745.6859	40.7817	3731.5487	51.6330

Table 14. β -PhXyl $\cdot$ (D₂O)₂

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	2.51	0.00
B	5.35	3.77
C	11.94	6.93
D	6.60	6.96



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	0.322153	-0.403425	-0.097225
6	1.435342	0.635639	-0.313454
6	2.737420	-0.098700	-0.642001
6	3.071279	-1.133027	0.426589
6	1.872483	-2.065703	0.610933
8	0.693373	-1.317777	0.927388
8	1.168231	1.509270	-1.391375
8	3.832528	0.806181	-0.738820
8	4.188479	-1.932812	0.060230
1	0.651664	2.282584	-1.065468
1	3.563580	1.505782	-1.359151
1	1.564854	1.195959	0.624446
1	2.607015	-0.620149	-1.604821
1	3.272636	-0.610286	1.374331
1	1.720402	-2.660194	-0.303364
1	2.033303	-2.749057	1.446984
1	4.905528	-1.330116	-0.198956
8	-0.845709	0.263690	0.322105
1	0.111589	-0.944851	-1.032738
6	-4.630087	-1.280783	-0.545484
6	-4.377995	0.094075	-0.599850
6	-3.103350	0.590330	-0.321738
6	-2.084844	-0.300661	0.022652
6	-2.320350	-1.675381	0.095856
6	-3.599183	-2.158266	-0.200806
1	-5.622265	-1.663855	-0.767848
1	-5.172328	0.784939	-0.869990
1	-2.883970	1.652417	-0.377506
1	-1.525411	-2.347642	0.399474
1	-3.788191	-3.227406	-0.147463
8	-0.169338	3.673627	-0.263845
1	-0.392912	3.440484	0.666767
1	0.244924	4.548135	-0.246278
8	-0.862311	2.448852	2.110693
1	-0.406113	2.342060	2.958105
1	-0.863530	1.568356	1.679629

B			
6	-0.006161	-0.282249	0.036835
6	1.307712	0.439636	0.387572
6	2.489835	-0.364435	-0.178189
6	2.401087	-1.830820	0.251108
6	1.031327	-2.405726	-0.100150
8	0.005769	-1.615210	0.509307
8	1.330781	1.753422	-0.170719
8	3.750608	0.110716	0.267237
8	3.393488	-2.610347	-0.398762
1	0.798064	2.347779	0.404503
1	3.987933	0.911942	-0.250706
1	1.398767	0.487895	1.481371
1	2.440373	-0.322947	-1.278631
1	2.536114	-1.878023	1.343101
1	0.899070	-2.438309	-1.192751
1	0.913991	-3.416664	0.294961
1	4.232542	-2.127508	-0.298565
8	-1.084424	0.385212	0.668135
1	-0.165262	-0.270462	-1.054197
6	-4.943560	-0.342691	-0.767411
6	-4.205685	0.741242	-1.252025
6	-2.908010	0.972723	-0.786388
6	-2.362374	0.110112	0.165128
6	-3.086615	-0.974298	0.661331
6	-4.382395	-1.196908	0.187431
1	-5.952502	-0.519889	-1.130132
1	-4.638299	1.410485	-1.991042
1	-2.321354	1.813581	-1.145959
1	-2.630501	-1.625589	1.398939
1	-4.953974	-2.039879	0.567030
8	-0.467657	2.977892	1.548708
1	-0.321739	3.176949	2.485364
1	-0.927640	2.115392	1.509236
8	3.778692	2.431707	-1.277081
1	2.845000	2.452668	-0.969157
1	4.190402	3.255949	-0.979423

C			
6	0.139451	0.213308	-0.395473
6	-1.062136	-0.559196	-0.943678
6	-2.312794	0.333451	-1.035978
6	-2.547421	1.190523	0.213570
6	-1.246961	1.874211	0.626083
8	-0.230870	0.877137	0.825820
8	-0.715701	-1.062744	-2.226054
8	-3.462248	-0.451579	-1.348732
8	-3.518081	2.201045	-0.031063
1	-1.526493	-1.433520	-2.614243
1	-3.596614	-1.081005	-0.604531
1	-1.253474	-1.390358	-0.251734
1	-2.182537	1.012290	-1.888723
1	-2.880593	0.544798	1.038085
1	-0.926938	2.594275	-0.141256
1	-1.354346	2.400926	1.576501
1	-4.283059	1.771065	-0.450271
8	1.146120	-0.701417	-0.090615
1	0.497419	0.961577	-1.118716
6	5.179810	0.374471	0.036967
6	4.212009	1.352445	0.273021
6	2.849293	1.034887	0.241933
6	2.463863	-0.277784	-0.045755
6	3.423664	-1.267265	-0.281864
6	4.777871	-0.938156	-0.235901
1	6.235485	0.629404	0.067825
1	4.511737	2.373264	0.496401
1	2.105502	1.790712	0.467724
1	3.091680	-2.275757	-0.509496
1	5.521183	-1.708704	-0.423847
8	-1.206036	-1.221395	2.549224
1	-0.768593	-0.489363	2.060368
1	-0.503669	-1.865974	2.725886
8	-3.404225	-2.087032	1.025873
1	-4.145079	-2.393272	1.568963
1	-2.673191	-1.857851	1.647884

D			
6	-0.160922	-0.055612	-0.061147
6	1.026269	0.909458	0.060974
6	2.289655	0.225719	-0.472094
6	2.534876	-1.123653	0.210699
6	1.246295	-1.952255	0.130410
8	0.123935	-1.240135	0.659674
8	0.876623	2.105724	-0.687643
8	3.408359	1.101302	-0.271792
8	3.540731	-1.890970	-0.423065
1	0.293698	2.719630	-0.189678
1	3.119482	1.982112	-0.572021
1	1.162268	1.132434	1.129821
1	2.167433	0.048165	-1.551645
1	2.784422	-0.944093	1.267767
1	1.060957	-2.240719	-0.915907
1	1.342370	-2.860665	0.727206
1	4.419470	-1.502193	-0.217441
8	-1.306244	0.542627	0.514905
1	-0.370480	-0.293990	-1.116884
6	-5.062736	-1.004301	-0.478661
6	-4.614056	0.188568	-1.052988
6	-3.349094	0.690825	-0.733806
6	-2.544732	-0.009797	0.165980
6	-2.980900	-1.198382	0.754583
6	-4.244838	-1.693824	0.422164
1	-6.045914	-1.393499	-0.729331
1	-5.246101	0.730903	-1.751266
1	-2.983814	1.616566	-1.169459
1	-2.333380	-1.716083	1.453243
1	-4.591370	-2.619921	0.873547
8	-1.040196	3.310162	0.944522
1	-0.926480	3.687708	1.829158
1	-1.353011	2.391265	1.064399
8	5.780778	-0.280585	0.116693
1	5.139696	0.442285	-0.053349
1	6.449958	-0.225367	-0.581202

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm ⁻¹	Intensity / km mol ⁻¹	Frequency / cm ⁻¹	Intensity / km mol ⁻¹	Frequency / cm ⁻¹	Intensity / km mol ⁻¹
v1	17.1699	0.5412	17.9750	0.3106	24.6524	0.1023
v2	28.8322	1.3639	28.1416	0.4301	33.4653	1.2052
v3	40.1475	1.7380	45.2029	2.3393	44.2516	0.6731
v4	48.5462	0.1298	51.6975	1.4107	48.7034	4.2696
v5	57.5997	0.6266	55.0431	2.6848	71.6692	1.0718
v6	60.2780	0.3016	95.7880	2.3469	79.7020	3.7497
v7	115.4177	3.0160	107.2795	2.0673	108.5889	7.0483
v8	116.3777	3.0430	125.1341	4.2752	117.4608	4.0441
v9	149.9700	13.4381	151.8646	4.5147	138.7080	49.0142
v10	162.7670	13.2983	159.9346	12.3295	149.4447	1.8255
v11	169.1070	18.9722	178.3071	3.1315	175.9175	4.9315
v12	186.0540	78.3000	196.3749	58.5572	194.0347	57.2967
v13	215.3412	3.3230	203.7752	88.3761	208.2696	9.3197
v14	224.0144	13.4167	226.8550	4.3482	225.4222	23.1815
v15	239.8949	15.0782	230.9605	43.8626	231.7580	25.7514
v16	251.8909	65.4829	246.0040	5.7011	251.9730	9.6774
v17	255.4818	1.2328	260.6539	20.3093	258.9722	2.8957
v18	268.2613	8.3817	281.6940	12.8615	282.0559	0.7160
v19	298.7319	24.4167	311.8557	28.6696	293.3407	25.3883
v20	302.0463	19.7178	321.5140	12.3374	320.6347	1.8067
v21	332.6480	0.9744	347.2454	13.2098	330.0608	2.0714
v22	377.6933	81.7266	383.4933	8.0303	352.2566	50.7080
v23	389.3199	113.8129	410.1444	6.4617	371.2511	68.0910
v24	408.1866	3.7735	424.0452	0.7367	404.4719	79.2489
v25	422.8098	0.0351	429.6599	71.4711	413.5793	54.1490
v26	435.1267	103.0186	445.0791	65.0698	422.3581	0.0710
v27	453.7079	10.4265	457.0634	57.1413	457.9435	0.0266
v28	461.2232	8.9432	461.7236	80.8903	470.2181	11.6290
v29	469.5405	6.3736	480.5775	26.8516	503.8877	56.6793
v30	519.4281	15.6098	522.7402	9.0776	518.8600	8.7478
v31	529.0412	25.1543	533.8166	13.8616	535.3187	7.7506
v32	545.1211	35.6151	543.1897	8.1063	542.9789	7.6591
v33	551.1704	34.4200	577.8559	13.0500	563.5297	38.0288
v34	574.2069	6.9385	627.7733	1.2562	584.1453	46.9024
v35	625.1987	3.0923	640.6118	23.4846	625.1610	1.1018
v36	646.2700	13.5349	659.5054	8.9964	646.1351	7.5144
v37	666.4203	18.0942	705.4388	38.8436	666.9259	10.1098
v38	703.6294	29.7389	764.0093	114.1855	701.0139	25.2034
v39	754.9059	116.3810	783.2360	50.7504	757.9003	144.5235
v40	774.2600	62.1573	791.2993	114.3283	768.4770	60.7383
v41	840.8358	15.3628	841.5979	16.5526	835.8093	6.8434
v42	846.7811	3.7327	846.6748	0.2894	840.7403	10.2345
v43	908.3385	4.9322	911.5694	5.4902	909.0228	3.6359
v44	922.1927	5.1171	930.4613	5.2318	910.3633	16.6531
v45	977.3748	0.0877	978.6822	0.5478	965.4880	128.9973
v46	989.1527	44.6620	999.2919	2.4874	971.3523	3.2647
v47	996.6368	0.7092	1003.5515	36.5076	993.1947	0.4072
v48	1015.9903	30.1676	1015.1733	78.5798	1014.8705	9.9324
v49	1023.3513	141.3380	1021.5560	29.3987	1024.5897	122.4175
v50	1047.0022	36.5488	1045.8144	5.6092	1042.6146	99.6855
v51	1049.2786	98.7378	1049.1802	229.9052	1051.8931	26.3734
v52	1058.6582	48.4605	1050.4879	26.7638	1061.7662	66.8228
v53	1094.7187	275.5741	1098.7029	110.8466	1077.1952	168.0544
v54	1105.9279	11.7247	1102.0920	105.6524	1096.9417	74.2031
v55	1109.0430	23.2338	1102.4828	109.9365	1105.0003	30.0968
v56	1115.9231	15.5195	1111.3356	69.5544	1111.7623	56.4906
v57	1129.9685	149.8411	1127.9531	79.9389	1128.2368	50.0918
v58	1142.7804	25.2791	1135.8426	27.8911	1139.0489	56.6205
v59	1153.0525	39.2833	1160.2833	5.3669	1158.7961	5.7595
v60	1189.4066	1.1269	1189.3284	0.3430	1187.8355	2.3920
v61	1199.2910	19.2477	1193.1111	15.4624	1200.6419	16.9685
v62	1224.9661	84.0289	1218.8213	54.6039	1239.1054	9.6079
v63	1229.2864	28.8725	1224.8850	81.0025	1244.3557	110.9707
v64	1248.2585	221.6312	1232.8147	92.0806	1252.8495	107.6662
v65	1252.1187	25.9112	1243.2112	36.1810	1261.9960	52.4655
v66	1257.5592	29.8543	1267.2174	41.8523	1266.0285	161.4067
v67	1277.9847	20.5029	1286.3569	17.9478	1285.3621	69.2721
v68	1298.9430	30.2051	1301.8040	17.5749	1294.9017	40.7662
v69	1321.5742	11.8311	1328.6975	9.2075	1312.4262	8.0183
v70	1344.7876	2.0650	1336.0495	2.1003	1338.9328	4.7402
v71	1360.8031	4.7978	1358.4062	1.0637	1346.0588	2.0619
v72	1364.3158	4.9067	1361.9741	1.3264	1364.5022	1.4115
v73	1367.6122	16.8113	1383.6245	13.6062	1371.2439	38.7455
v74	1390.1907	37.0207	1399.0307	54.8769	1383.9759	44.0840
v75	1402.8867	42.4891	1414.1963	50.2616	1405.5036	15.2063

v76	1426.0253	19.7401	1422.3550	8.6207	1427.9616	2.5309
v77	1439.1871	23.1603	1444.5276	18.4212	1442.8963	4.2209
v78	1450.6058	3.2988	1468.7160	28.7724	1460.2169	43.5325
v79	1482.9336	15.8439	1490.7052	20.1606	1489.7573	38.9665
v80	1497.9231	0.8567	1493.4095	1.8785	1497.6578	0.6168
v81	1524.0071	4.4249	1524.8220	3.5102	1524.8444	6.1200
v82	1534.9032	91.3939	1533.6216	64.8339	1535.1688	100.2275
v83	1642.1544	21.0545	1642.7427	4.8453	1639.6988	22.3166
v84	1650.2940	46.9612	1645.4922	34.8692	1652.2608	61.3539
v85	2534.4823	209.1840	2560.4895	227.3090	2512.2456	268.6660
v86	2602.5915	224.0541	2624.3068	112.0167	2572.3623	193.7620
v87	2793.5745	99.9547	2791.2808	87.5316	2777.5738	71.5132
v88	2794.0897	71.4886	2796.7166	111.1920	2788.9549	68.3271
v89	2995.4902	5.9768	2994.6935	9.2876	3025.4606	8.7506
v90	3010.3267	4.8032	3001.7435	7.4138	3031.3610	10.4059
v91	3014.5171	2.6004	3009.2182	8.5714	3041.9070	28.6929
v92	3023.5716	37.5668	3025.4584	72.2042	3051.7388	3.3908
v93	3036.8301	104.2750	3051.5785	45.5476	3069.1320	71.2705
v94	3142.8253	19.9170	3142.4080	20.5865	3142.6146	16.6247
v95	3185.3245	0.3420	3185.4407	0.2003	3183.9429	0.9025
v96	3194.6786	15.1928	3194.6524	11.3947	3192.3527	14.6104
v97	3207.4838	24.5421	3205.0197	23.2083	3206.8701	27.7115
v98	3216.9598	4.4157	3212.6128	10.2770	3216.0249	6.9478
v99	3229.6517	1.1418	3230.8627	1.6184	3228.6355	3.0609
v100	3474.4207	716.2210	3501.4131	593.1404	3523.6729	328.5573
v101	3718.1099	47.3060	3513.4742	608.1072	3719.5341	12.1332
v102	3731.7326	49.6609	3710.1861	49.5534	3721.3411	80.8639

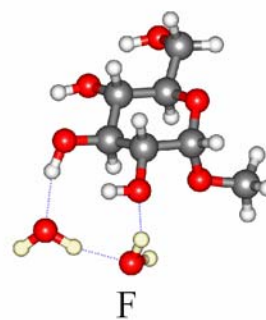
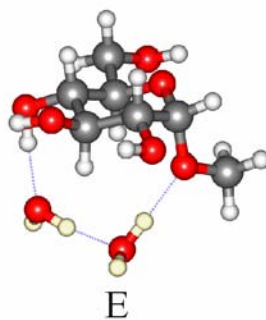
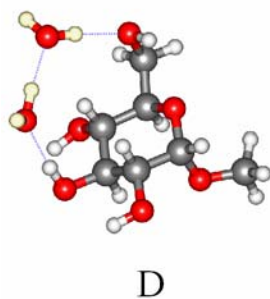
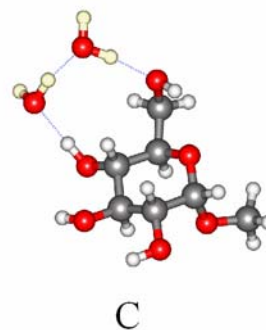
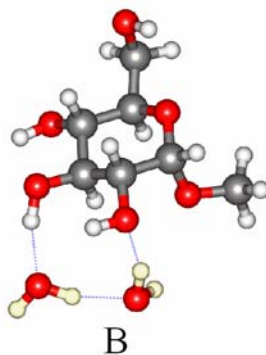
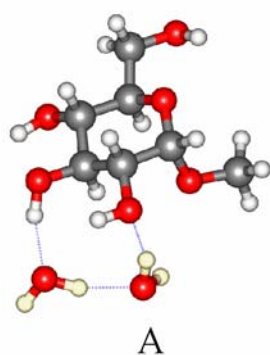
D		
	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	14.4492	0.2399
v2	27.3359	1.8138
v3	42.4066	1.3009
v4	51.9085	1.9496
v5	55.5514	2.5043
v6	98.8226	3.5155
v7	105.9082	6.0398
v8	130.9648	12.1801
v9	150.6382	4.8996
v10	162.2780	4.6806
v11	173.0822	4.5855
v12	190.6374	69.5972
v13	210.0039	81.9332
v14	229.2663	32.1860
v15	232.8541	18.3176
v16	243.0725	2.5138
v17	263.4529	16.8126
v18	278.0455	32.8364
v19	301.6869	13.4313
v20	326.6333	13.4196
v21	335.9985	3.5647
v22	366.3989	2.7623
v23	407.7771	2.7508
v24	424.8591	1.1965
v25	439.7061	14.0224
v26	454.5131	49.7086
v27	458.6410	113.3462
v28	477.0073	19.9052
v29	488.9492	96.8056
v30	520.2889	18.4549
v31	533.4441	36.4724
v32	542.1582	12.6809
v33	581.6744	10.0085
v34	626.7305	2.8277
v35	644.5360	18.9324
v36	661.6217	15.6013
v37	706.2769	38.1895
v38	747.8166	123.4751
v39	763.7104	104.8270
v40	786.7781	50.7699
v41	841.3957	14.2112
v42	848.4913	0.5845
v43	899.5936	2.7636
v44	932.2305	5.4466
v45	980.5855	0.8874
v46	999.7049	11.6228
v47	1002.0646	21.2709
v48	1016.3623	66.7115
v49	1024.2431	127.9639
v50	1045.6300	59.4985
v51	1048.7089	55.0850
v52	1059.2689	31.1721
v53	1096.7040	165.2421
v54	1101.8195	1.8597
v55	1106.3902	186.4809
v56	1113.9597	29.2783
v57	1128.0644	126.2360
v58	1142.1581	42.5253
v59	1146.0917	10.5563
v60	1189.4360	0.0815
v61	1194.0349	17.0607
v62	1216.7568	50.3355
v63	1223.3757	64.0694
v64	1232.6192	106.4658
v65	1240.6305	67.6914
v66	1269.6170	23.9045
v67	1287.1554	37.2948
v68	1321.7137	11.5046
v69	1326.9310	15.2754
v70	1336.8889	3.0222
v71	1358.9427	0.4901
v72	1364.7492	16.4970
v73	1367.1956	27.3802
v74	1394.3547	72.5330
v75	1402.6697	10.5648

v76	1424.6301	19.6316
v77	1440.8454	16.4675
v78	1462.1939	14.0604
v79	1484.0972	24.8785
v80	1493.8460	1.6831
v81	1520.1828	5.1134
v82	1533.5711	69.1200
v83	1641.7495	7.6994
v84	1645.9146	34.3343
v85	2590.1413	174.6834
v86	2623.5785	116.4889
v87	2792.4754	97.8568
v88	2797.1218	105.3568
v89	2998.4070	13.2785
v90	3012.4188	1.5209
v91	3015.7323	2.0965
v92	3025.0926	18.6534
v93	3038.5021	106.5048
v94	3149.7004	18.0056
v95	3185.3811	0.1644
v96	3194.7302	12.6602
v97	3205.5815	23.4293
v98	3213.3855	8.9260
v99	3236.5259	0.9229
v100	3521.4298	682.6823
v101	3535.2896	496.6512
v102	3695.2835	60.6583

Table 15. α -MeGlu $\cdot$ (D₂O)₂

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	3.38	0.00
B	4.34	0.21
C	2.15	0.27
D	7.68	1.14
E	10.26	1.24
F	3.30	1.92



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	-0.407370	1.233593	0.863480
6	0.629812	0.177847	1.261486
6	0.645308	-0.965414	0.241730
6	-0.760253	-1.560431	0.137381
6	-1.758258	-0.458848	-0.234556
8	-1.678298	0.617522	0.731259
8	1.907367	0.806659	1.400105
8	1.552123	-1.989277	0.636275
8	-0.813691	-2.572651	-0.858484
6	-3.209752	-0.922552	-0.216781
8	-4.104223	0.128906	-0.561522
1	2.527327	0.130420	1.724728
1	2.389537	-1.867567	0.134709
1	-3.953640	0.849835	0.071365
1	-0.538896	1.977363	1.660157
1	0.323397	-0.223525	2.236723
1	0.932138	-0.575193	-0.742720
1	-1.037230	-1.982229	1.117794
1	-1.516539	-0.068034	-1.231243
1	-0.058578	-3.162829	-0.689931
1	-3.451809	-1.331483	0.776477
1	-3.347324	-1.710338	-0.960368
8	0.024123	1.864453	-0.318057
6	-0.733490	3.023068	-0.669446
1	-0.250088	3.457140	-1.547380
1	-1.769313	2.762253	-0.914008
1	-0.722054	3.754887	0.150506
8	3.803997	-1.162992	-0.738869
1	3.691226	-0.216195	-1.004490
1	4.462003	-1.558971	-1.327421
8	3.151544	1.482194	-1.025673
1	2.642797	1.460749	-0.182851
1	2.497523	1.741621	-1.692080

B			
6	-0.283454	1.375315	0.716081
6	0.499879	0.151953	1.200173
6	0.434970	-0.966840	0.157107
6	-1.030055	-1.312969	-0.109813
6	-1.800723	-0.057634	-0.537807
8	-1.620454	1.002677	0.431146
8	1.842075	0.545884	1.501641
8	1.110204	-2.131972	0.620206
8	-1.142181	-2.263484	-1.163094
6	-3.310483	-0.265323	-0.633460
8	-3.899104	-0.578897	0.622326
1	2.299480	-0.241275	1.846246
1	2.008705	-2.147444	0.220652
1	-3.670120	0.139792	1.234253
1	-0.366460	2.129786	1.509094
1	0.016847	-0.196990	2.122835
1	0.890354	-0.621957	-0.779706
1	-1.478297	-1.715333	0.810369
1	-1.424372	0.269569	-1.517212
1	-0.565994	-3.009612	-0.924424
1	-3.515911	-1.109156	-1.296214
1	-3.767243	0.639750	-1.061553
8	0.377579	1.923684	-0.400362
6	-0.105504	3.212053	-0.781842
1	-1.158868	3.169428	-1.081676
1	0.503498	3.536173	-1.628628
1	0.010117	3.927988	0.044053
8	3.633898	-1.678371	-0.427847
1	4.259921	-2.183338	-0.965883
1	3.705782	-0.727996	-0.695916
8	3.453391	1.034803	-0.742084
1	2.928857	1.398558	-1.471189
1	2.852673	1.088136	0.036807

C			
6	-2.033736	-0.514222	0.591386
6	-1.631542	0.932478	0.901202
6	-0.732234	1.472857	-0.205529
6	0.496620	0.576769	-0.375412
6	0.038130	-0.873551	-0.621748
8	-0.852012	-1.308284	0.430231
8	-2.797774	1.714941	1.088698
8	-0.364629	2.799941	0.168675
8	1.252252	1.059221	-1.477565
6	1.162710	-1.901578	-0.628943
8	1.745833	-2.063811	0.673550
1	-2.511832	2.643809	1.114109
1	0.264725	3.120472	-0.499505
1	1.008421	-2.112545	1.307752
1	-2.551210	-0.966189	1.447369
1	-1.047141	0.903603	1.834826
1	-1.290565	1.496259	-1.151874
1	1.091444	0.622161	0.547529
1	-0.477655	-0.915511	-1.590495
1	2.199012	1.141498	-1.217433
1	0.775714	-2.869902	-0.971557
1	1.962997	-1.581406	-1.300033
8	-2.840260	-0.542798	-0.546016
6	-3.549584	-1.762779	-0.738885
1	-2.865901	-2.605310	-0.903205
1	-4.191195	-1.978913	0.127427
1	-4.174262	-1.620120	-1.623193
8	4.056338	-0.694029	1.284736
1	4.774540	-1.301923	1.511220
1	3.251862	-1.244206	1.131271
8	3.877506	1.270409	-0.630056
1	4.087875	0.601339	0.065317
1	4.572951	1.202322	-1.299981

D			
6	1.750175	-0.020305	-0.827579
6	0.909031	1.245473	-0.627551
6	0.262669	1.225663	0.760173
6	-0.559851	-0.051277	0.932754
6	0.250085	-1.306430	0.582543
8	0.898791	-1.165475	-0.696876
8	1.710358	2.396374	-0.825488
8	-0.539126	2.387040	0.977526
8	-1.020296	-0.205529	2.274008
6	-0.627916	-2.547816	0.445470
8	-1.503923	-2.454011	-0.690007
1	1.244045	3.136438	-0.398681
1	-1.325354	2.344609	0.385605
1	-0.937946	-2.265570	-1.459292
1	2.132674	-0.082155	-1.854736
1	0.112648	1.210318	-1.388653
1	1.048799	1.265643	1.521081
1	-1.419121	0.005834	0.253394
1	0.996880	-1.477634	1.369145
1	-1.350819	0.662261	2.563452
1	0.001350	-3.441080	0.342832
1	-1.263396	-2.656430	1.326629
8	2.797304	-0.036659	0.093814
6	3.825855	-0.979119	-0.194195
1	4.592905	-0.842509	0.571001
1	4.262250	-0.785470	-1.184544
1	3.449988	-2.009513	-0.158682
8	-3.628516	-0.646540	-1.018917
1	-4.428674	-0.953705	-0.567949
1	-2.935371	-1.327269	-0.849261
8	-2.814776	2.001044	-0.689812
1	-3.159176	1.087251	-0.833796
1	-3.080508	2.521904	-1.461217

E			
6	-0.231732	1.487937	-0.856606
6	-1.160381	0.431711	-1.466253
6	-0.970329	-0.924513	-0.795531
6	0.505268	-1.338479	-0.758193
6	1.366881	-0.199736	-0.185108
8	1.106380	1.033808	-0.901483
8	-2.504660	0.884893	-1.381214
8	-1.760733	-1.859436	-1.530956
8	0.661517	-2.555244	-0.042070
6	2.862501	-0.449583	-0.332168
8	3.635255	0.607126	0.226242
1	-3.062038	0.184176	-1.759671
1	-1.549666	-2.746563	-1.192264
1	3.378435	1.422479	-0.234256
1	-0.244803	2.401867	-1.462381
1	-0.860402	0.336085	-2.520763
1	-1.347338	-0.866284	0.233792
1	0.832813	-1.551297	-1.783707
1	1.131061	-0.048759	0.876460
1	0.354500	-2.419798	0.884461
1	3.134467	-1.358669	0.208310
1	3.105838	-0.591266	-1.396492
8	-0.649269	1.800303	0.459128
6	-0.020592	2.961538	1.013524
1	1.057013	2.807204	1.133404
1	-0.202831	3.833188	0.371312
1	-0.479187	3.126687	1.990489
8	-1.884120	0.325149	2.491204
1	-2.842640	0.241216	2.376050
1	-1.565254	0.853694	1.725955
8	-0.372993	-2.005284	2.535040
1	-0.930519	-1.195784	2.626449
1	0.129829	-2.091948	3.357734

F			
6	-0.059182	1.494867	0.832978
6	0.722428	0.249243	1.267770
6	0.406375	-0.929698	0.340805
6	-1.103862	-1.153588	0.349490
6	-1.828645	0.126715	-0.086724
8	-1.446563	1.203613	0.792627
8	2.117913	0.562065	1.304749
8	1.051893	-2.119971	0.780168
8	-1.472332	-2.214336	-0.531836
6	-3.354469	0.011143	-0.010357
8	-3.879743	-0.801823	-1.048920
1	2.578621	-0.215131	1.665666
1	1.864367	-2.244628	0.239734
1	-3.382437	-1.639216	-1.052474
1	0.034250	2.296099	1.577207
1	0.388008	-0.003179	2.282911
1	0.723090	-0.691344	-0.682055
1	-1.418205	-1.404738	1.375420
1	-1.547327	0.369660	-1.119958
1	-0.883287	-2.962663	-0.329921
1	-3.792542	1.005405	-0.136947
1	-3.647997	-0.364684	0.982788
8	0.446685	1.927506	-0.407790
6	-0.027694	3.213608	-0.809966
1	0.477910	3.453067	-1.747990
1	-1.111994	3.206450	-0.967782
1	0.226456	3.971614	-0.055929
8	3.340434	-1.960202	-0.761489
1	3.448296	-1.032277	-1.088982
1	3.876919	-2.536955	-1.323325
8	3.342326	0.740774	-1.214792
1	2.735578	1.114342	-1.871678
1	2.895688	0.903421	-0.352399

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	29.5498	2.3621	20.5059	4.3865	25.2050	1.5603
v2	44.5336	5.6111	46.2832	0.6722	30.3871	1.5974
v3	51.2792	9.4826	54.6560	4.2150	50.1577	0.0609
v4	68.7391	9.3096	69.2041	6.8908	72.8338	1.1686
v5	76.1165	1.9606	80.0164	0.8170	77.2219	7.2096
v6	81.7787	40.7180	92.6065	21.4761	102.0411	2.8050
v7	111.2764	4.1604	106.5832	20.8324	113.3885	4.5196
v8	120.1158	5.6246	121.0414	0.9524	124.4660	0.6865
v9	132.6983	0.7277	122.4329	12.9093	145.6156	55.4799
v10	158.6582	6.4864	150.0914	3.4571	157.7685	2.5215
v11	178.0317	2.1032	186.5299	13.4026	174.3014	28.8728
v12	199.3858	28.8661	195.9245	33.4879	203.1872	58.3845
v13	205.1874	5.9620	217.4919	12.3070	209.4402	12.1352
v14	221.1321	13.8207	227.8926	14.3932	221.7863	0.7948
v15	238.8842	23.8270	239.6037	16.0479	236.5784	5.4659
v16	243.5751	9.8548	248.4619	28.8688	252.9018	16.2935
v17	257.0777	22.1235	255.9125	8.3533	255.7823	33.3878
v18	270.2629	34.3538	268.7496	18.2663	269.9149	20.9203
v19	276.6124	30.4649	276.2295	25.0398	280.6035	1.3036
v20	302.9235	6.5510	283.2099	25.2895	310.2285	41.4731
v21	334.3180	13.8156	324.6823	11.2648	323.9813	4.5208
v22	358.1971	8.5317	344.6009	11.0133	347.6650	11.3108
v23	375.0711	55.7162	379.1799	75.7210	369.3055	137.6825
v24	400.0416	33.4718	394.0374	28.2491	379.5587	16.3311
v25	413.0804	44.6472	408.7601	133.9939	395.4858	40.3939
v26	426.8639	210.9041	415.4057	101.2965	408.2615	59.6708
v27	436.5482	7.4841	444.0777	42.0033	431.2913	3.8484
v28	448.0322	19.0677	468.2340	125.5542	459.3711	148.9537
v29	478.0177	161.8988	504.6725	8.5019	504.1070	6.5846
v30	545.0048	5.5329	532.9254	31.0212	523.5918	10.7397
v31	569.1981	23.7452	560.1675	4.5088	543.9200	55.2515
v32	578.7325	86.5534	579.1788	67.7439	557.6789	19.4708
v33	592.6775	34.7534	595.2172	105.5579	609.4422	4.9962
v34	604.7995	31.5643	616.5663	7.9303	629.1872	67.9153
v35	666.0316	13.1029	707.1693	11.7812	708.9815	14.8614
v36	753.0490	11.6697	755.9347	6.5758	755.5175	77.4115
v37	780.1203	27.0253	772.9881	30.9127	760.8907	43.0010
v38	835.2718	28.6896	868.1051	14.9308	869.5516	23.6766
v39	909.5596	26.6797	911.4700	26.4521	911.0942	4.9010
v40	1007.9872	41.6680	919.9068	22.8447	921.9720	16.4334
v41	1016.8005	112.1389	1013.7057	47.4799	1010.6522	82.5836
v42	1029.6249	30.7404	1020.7928	36.0562	1022.5690	233.8960
v43	1056.3166	16.1046	1038.2645	194.0735	1038.0530	160.1190
v44	1059.1893	295.8752	1064.7275	61.9908	1061.3905	64.0803
v45	1073.4268	83.2137	1068.9565	266.9657	1066.3308	153.5693
v46	1091.6213	148.1928	1102.1140	60.3387	1098.5254	6.1083
v47	1114.5944	27.1530	1108.0975	91.2156	1118.1470	51.7473
v48	1124.1360	50.6076	1122.7342	17.6102	1123.6862	58.7790
v49	1136.0184	42.2595	1135.7978	62.0547	1132.5694	3.5421
v50	1150.2755	33.7726	1140.2672	5.9184	1142.2759	78.4090
v51	1157.5872	106.5405	1157.2334	124.0920	1162.2997	127.9809
v52	1183.8804	2.0371	1182.3999	2.0280	1182.4710	3.2769
v53	1209.3437	23.6638	1210.7291	16.4872	1206.6978	44.5159
v54	1223.9001	9.9759	1228.7026	16.7850	1234.3034	1.3123
v55	1237.2814	79.2912	1237.9555	77.9897	1237.3228	51.3973
v56	1245.8062	22.2623	1247.4754	9.2193	1247.5981	30.9059
v57	1251.8815	8.8758	1253.7293	24.4694	1255.0836	31.2117
v58	1274.4446	35.8988	1273.7677	29.6295	1266.6562	4.4101
v59	1279.4256	34.2537	1278.4785	40.0164	1272.3199	28.7421
v60	1316.2913	8.7035	1317.1425	4.6533	1315.9752	36.2712
v61	1350.7628	11.5508	1346.9781	0.8635	1338.6443	9.6170
v62	1357.9941	1.3176	1358.2649	22.7714	1359.0100	12.5471
v63	1371.9402	25.4228	1370.6552	14.0345	1365.4271	14.0321
v64	1393.7889	9.0535	1388.2660	10.9225	1378.0405	12.7504
v65	1399.3869	5.4900	1400.9287	13.4820	1403.0995	12.9467
v66	1407.9333	46.8228	1410.2402	37.7482	1408.4881	41.8396
v67	1419.6397	9.2395	1422.8225	23.5800	1426.5092	10.9741
v68	1434.4701	42.5997	1432.7767	41.0628	1438.1314	43.9779
v69	1438.9562	13.4150	1437.6410	3.7967	1443.6326	15.3792
v70	1454.1647	8.1245	1454.4673	7.5088	1449.9599	20.9054
v71	1475.6573	13.4986	1473.2026	13.1947	1490.3357	18.0921
v72	1494.0784	3.3981	1493.3390	2.8212	1493.6375	3.4987
v73	1507.9399	5.7598	1506.3863	5.3096	1509.3045	5.4162
v74	1517.3567	2.0678	1514.0502	7.3355	1518.0762	7.6495
v75	1530.0009	6.6218	1528.9190	6.9155	1527.1537	6.0369

v76	2470.4986	274.4378	2467.4890	271.7806	2492.6514	295.1978
v77	2560.0522	246.1838	2556.2221	253.1538	2532.9168	367.0690
v78	2780.0282	46.9126	2779.9023	45.5139	2787.8351	61.5849
v79	2795.0978	69.0871	2793.4864	67.2991	2792.4318	88.5045
v80	2993.3360	18.0647	3017.1044	46.0359	3000.9762	26.4766
v81	3014.5859	47.1771	3028.1692	57.0848	3021.3011	60.7119
v82	3028.5259	54.0279	3031.0914	3.1355	3034.2659	0.8425
v83	3044.3365	14.6226	3042.7813	11.8099	3045.0784	22.8194
v84	3057.9924	43.9013	3046.6139	35.5280	3051.5099	12.4208
v85	3062.2505	3.5001	3058.2670	34.8079	3059.2614	45.2626
v86	3070.6477	61.8457	3067.9020	61.0652	3062.5003	80.9840
v87	3100.5234	28.3683	3097.7264	30.8409	3082.7193	38.9592
v88	3144.6843	10.3496	3139.6191	9.4434	3140.7688	12.8718
v89	3151.4993	21.1718	3150.4873	21.5971	3151.9146	22.1467
v90	3506.2571	680.3508	3509.8032	668.8300	3464.0025	900.4380
v91	3710.9022	38.3818	3714.8873	46.8929	3708.5732	61.3155
v92	3718.1816	59.8744	3723.2598	51.4659	3725.7165	46.0794
v93	3739.5280	24.9408	3738.3258	25.5727	3727.2929	52.0525

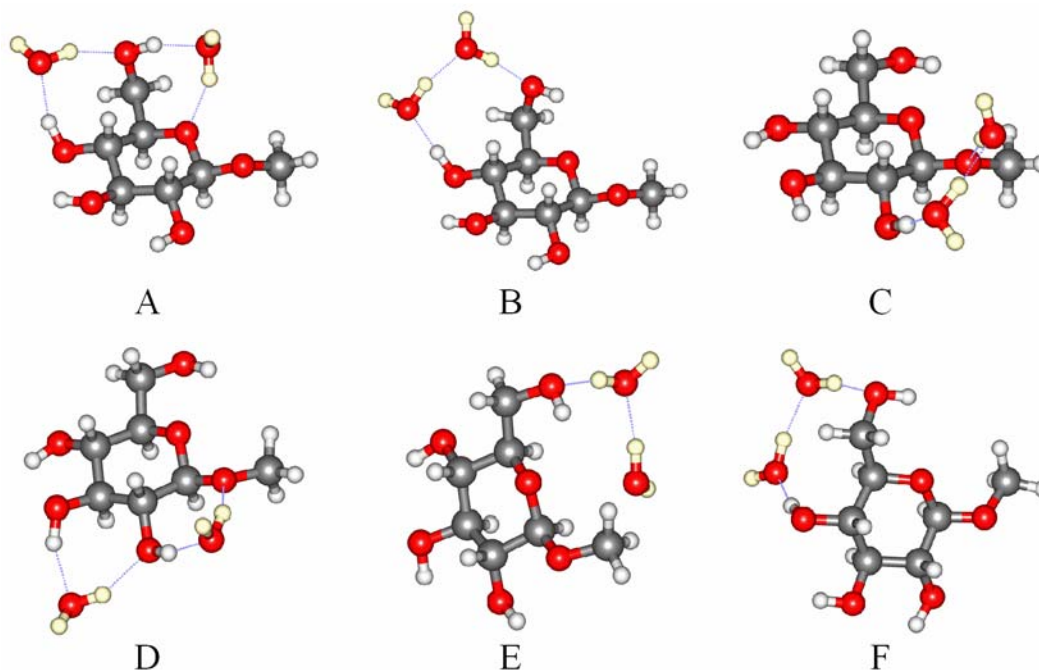
	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	35.5674	1.2701	29.3991	0.8484	28.7527	1.5878
v2	42.1452	0.8052	43.2662	0.4475	33.8546	34.8443
v3	64.6487	1.5985	65.9138	1.8436	47.6826	7.8949
v4	71.2000	5.9343	71.9390	2.8465	62.1078	9.3850
v5	77.7628	2.5484	82.7143	2.0258	73.3566	14.4285
v6	100.3679	22.3955	105.1798	3.4048	77.7612	6.6176
v7	109.7148	5.0841	114.1716	14.7437	112.1465	0.1368
v8	122.0868	5.8637	123.6114	0.1833	117.6363	3.8998
v9	123.5856	32.3627	149.6295	46.3027	148.2727	2.6213
v10	157.4524	2.7888	154.1789	0.3620	158.9101	11.7416
v11	164.6984	48.6333	168.4813	4.4602	181.4562	10.3463
v12	187.6506	29.8478	185.5531	2.9049	201.7001	6.9222
v13	207.2649	30.3412	193.5505	17.5827	215.8213	18.4325
v14	217.0774	7.8462	219.5515	105.7328	223.1562	11.1529
v15	233.5363	11.6972	227.9638	0.5784	235.9972	30.5247
v16	248.8238	11.8731	237.6169	25.8927	245.0403	9.0919
v17	256.4280	23.1481	250.0861	27.7910	264.2907	26.5439
v18	261.7139	8.7298	257.6770	25.9909	273.3879	32.2708
v19	271.3646	9.5775	277.8441	11.7654	282.1258	20.0968
v20	314.5323	40.9628	302.6311	3.7893	317.8508	4.5032
v21	322.5425	5.5001	333.6922	4.3800	328.2620	15.7948
v22	338.3096	6.1580	351.4126	13.0099	351.5123	8.2923
v23	350.6372	9.2771	359.7911	16.1597	374.1964	71.1355
v24	365.8303	32.7740	397.1736	49.3893	394.5696	9.9229
v25	402.9220	4.8116	399.8240	113.8613	424.5533	35.0139
v26	408.6461	146.0434	411.7093	89.7954	432.0142	50.0251
v27	433.6592	10.2949	414.3922	53.7066	461.0570	152.4028
v28	490.9160	147.2700	432.4319	21.1089	493.7562	22.9874
v29	508.6418	4.4399	444.6618	44.2619	500.9918	11.9263
v30	522.9916	38.1660	523.7930	83.7630	512.0641	153.9605
v31	549.3725	38.9864	542.8218	1.1173	562.1566	20.2824
v32	561.2088	8.8785	572.6379	9.0065	574.8814	92.0012
v33	590.5614	92.8398	608.0768	10.6956	586.7155	7.7082
v34	618.8008	26.4458	612.7275	75.8421	597.5504	47.2481
v35	712.4776	6.3454	667.2515	17.5239	659.9070	19.2128
v36	760.6578	11.2033	755.8554	19.3886	743.6914	11.9343
v37	805.3865	130.6609	775.1453	137.0956	767.0409	30.9051
v38	876.0910	24.1200	833.3099	18.0739	901.1985	10.3203
v39	912.8705	7.6011	904.2025	23.8346	903.1232	10.0255
v40	921.8202	37.5625	999.6668	100.2745	980.8473	46.4402
v41	1015.2625	27.6306	1020.0953	123.2717	1014.6895	32.8395
v42	1023.6342	310.1530	1031.8469	34.8043	1019.3290	119.2040
v43	1030.6244	23.7950	1054.1880	28.6592	1057.4339	65.2157
v44	1061.0078	108.1446	1060.9568	262.0699	1068.6217	239.3668
v45	1068.0651	161.8380	1079.0148	126.9670	1085.6449	204.0539
v46	1091.5997	39.0410	1092.8789	61.0789	1102.8929	62.6854
v47	1100.6677	67.1160	1115.4397	15.0659	1115.4385	16.8782
v48	1127.8508	12.9844	1118.4625	134.4468	1130.1729	69.1540
v49	1137.8748	13.5421	1131.3042	6.8658	1136.1174	23.0047
v50	1146.1435	66.7602	1148.9812	14.1501	1146.1237	23.2407
v51	1162.1904	131.5169	1155.5049	86.3259	1157.8899	107.5985
v52	1182.9205	3.9439	1182.0957	1.8038	1183.4171	1.6374
v53	1215.0123	35.1332	1212.4978	14.5193	1203.7197	14.5440
v54	1228.2528	34.4643	1228.8761	18.2206	1214.2540	7.0602
v55	1245.8032	54.5952	1236.9998	42.2124	1236.4913	76.1322
v56	1255.2004	14.2074	1246.0052	29.9081	1246.4230	16.4099
v57	1261.9433	6.1229	1252.9183	12.9236	1269.8662	44.1749
v58	1262.8889	35.3794	1268.7181	24.6241	1277.0964	23.9669
v59	1287.0617	47.9806	1274.3336	15.8340	1278.7891	33.8430
v60	1311.7534	33.4083	1297.8506	20.4020	1318.8931	0.4445
v61	1340.4428	11.1895	1350.2898	18.7543	1338.4262	5.8481
v62	1349.3600	11.2168	1362.0208	20.0530	1359.9255	5.1446
v63	1364.8847	5.1044	1375.2915	7.0000	1374.8247	13.0941
v64	1384.6167	2.9074	1394.1444	10.4499	1390.7341	27.2604
v65	1402.0628	24.8753	1396.7512	18.5212	1402.1340	17.2979
v66	1414.9056	20.0521	1406.5547	11.5779	1412.3679	20.6560
v67	1427.6218	5.6250	1412.7225	8.2108	1420.6128	23.7118
v68	1432.7605	17.3039	1439.0161	47.7584	1438.7933	2.6283
v69	1436.9297	51.1290	1447.0351	15.6554	1446.9016	12.7009
v70	1460.4086	10.9567	1454.2523	4.4078	1456.4535	75.8298
v71	1479.9439	39.3144	1484.4716	48.9839	1473.6317	13.9872
v72	1493.6334	2.9825	1493.6400	2.6416	1493.9458	3.0112
v73	1509.1633	5.3772	1508.0197	7.3838	1506.9489	5.6716
v74	1515.5624	7.6980	1517.6595	1.9976	1528.8010	5.8112
v75	1527.0510	6.2091	1528.5475	5.8372	1530.0359	2.9274

v76	2500.5198	363.3945	2505.3307	293.3345	2468.5056	277.8331
v77	2538.4867	238.4415	2570.2689	220.8320	2559.6141	246.1736
v78	2785.0305	81.1096	2782.6959	87.2274	2779.3589	47.2848
v79	2789.4611	61.7640	2789.3253	63.7133	2795.1672	69.3451
v80	2997.4217	32.8868	3016.0577	35.5839	2999.5454	0.6192
v81	3021.7777	58.7197	3021.3161	18.4247	3006.3017	65.7731
v82	3049.1479	11.4815	3038.8678	47.6055	3030.0103	55.5142
v83	3056.6020	50.6592	3051.5796	1.1222	3045.3414	13.7791
v84	3060.6983	32.2883	3057.3915	1.7804	3055.9446	24.1783
v85	3070.8064	29.9636	3071.5706	25.9126	3061.9829	34.2466
v86	3082.9935	39.2252	3073.9934	95.9488	3071.7070	52.6699
v87	3101.6010	30.0826	3111.0416	24.4409	3101.1307	28.8494
v88	3150.6569	8.0991	3143.6937	12.0879	3113.4892	29.1815
v89	3151.9590	21.8447	3159.4883	13.3385	3151.7192	21.1431
v90	3499.0788	430.1017	3487.3800	442.0225	3506.3378	676.4870
v91	3702.6741	40.1248	3720.5734	49.0451	3694.6547	129.7480
v92	3713.8200	48.8786	3730.8753	50.2370	3709.6498	14.5488
v93	3718.0708	49.4960	3740.7844	24.4619	3721.9019	54.7836

Table 16. β -MeGlu $\cdot$ (D₂O)₂

(a) Relative energies, with respect to those of the lowest energy conformer at 0 K, calculated at the B3LYP/6-31+G(d) and MP2/6-311++G(d,p)//B3LYP/6-31+G(d) level of theory. Corresponding optimized structures are provided as well.

Conformer	B3LYP/6-31+G(d) energy / kJ mol ⁻¹	MP2/6-311++G(d,p)//B3LYP/6-31+G(d) energy / kJ mol ⁻¹
A	0.00	0.00
B	2.28	6.16
C	4.75	7.79
D	7.39	9.46
E	12.76	11.13
F	10.02	11.29



(b) Cartesian coordinates of optimized geometries (in Å) of lowest energy conformers.

A			
6	-1.768887	-0.041174	-0.337841
6	-1.431446	1.227809	0.446539
6	-0.166548	1.870455	-0.120829
6	0.994070	0.880093	-0.179550
6	0.555102	-0.341801	-1.007972
8	-0.621266	-0.910387	-0.396765
8	-2.538771	2.111491	0.351727
8	0.135697	2.992615	0.701737
8	2.104157	1.557398	-0.751987
6	1.609267	-1.441096	-1.144233
8	2.227386	-1.839743	0.077442
1	-2.249437	2.968004	0.709185
1	0.999730	3.330009	0.407547
1	1.576646	-2.322547	0.639862
1	-1.253946	0.943252	1.494870
1	-0.377306	2.217728	-1.146427
1	1.234576	0.550125	0.839396
1	0.300997	-0.011475	-2.029271
1	2.921039	1.209394	-0.327735
1	2.411192	-1.063461	-1.784738
1	1.153938	-2.308514	-1.640606
8	-2.774268	-0.732768	0.315551
1	-2.067119	0.214931	-1.369005
6	-3.483859	-1.672995	-0.493063
1	-4.255858	-2.103628	0.147449
1	-2.822802	-2.468678	-0.856766
1	-3.958851	-1.166551	-1.344235
8	0.046593	-2.945055	1.377784
1	-0.491422	-2.248938	0.944124
1	-0.121477	-2.874439	2.329035
8	4.008930	0.142004	0.689125
1	4.935618	-0.051886	0.487844
1	3.510615	-0.705525	0.604257

B			
6	2.096285	-0.269885	0.122617
6	1.683089	1.047270	-0.536727
6	0.521136	1.663976	0.238631
6	-0.652407	0.696358	0.382412
6	-0.137567	-0.599506	1.036491
8	0.951952	-1.131489	0.269413
8	2.807175	1.915605	-0.536946
8	0.146307	2.855836	-0.445018
8	-1.637947	1.321715	1.191677
6	-1.160315	-1.728252	1.104791
8	-1.473303	-2.234852	-0.200926
1	2.482544	2.795945	-0.791381
1	-0.636940	3.208863	0.011155
1	-0.630176	-2.315187	-0.682971
1	1.364018	0.827472	-1.566589
1	0.874023	1.922536	1.251343
1	-1.054859	0.469179	-0.614022
1	0.190763	-0.367389	2.063090
1	-2.522246	1.234112	0.764560
1	-2.094348	-1.369099	1.543162
1	-0.766166	-2.544897	1.723363
8	3.014479	-0.916562	-0.682167
1	2.517343	-0.076895	1.125821
6	3.734730	-1.970017	-0.046548
1	4.464859	-2.324407	-0.776975
1	3.070100	-2.794068	0.238877
1	4.262685	-1.596996	0.842677
8	-3.728387	-1.308003	-1.482355
1	-2.929898	-1.720107	-1.074983
1	-4.335421	-2.027169	-1.707790
8	-4.057206	1.043567	-0.106842
1	-4.864691	1.058791	0.426857
1	-4.085859	0.213110	-0.640883

C			
6	-0.312117	-0.593049	-0.670374
6	-0.676380	0.832144	-0.227399
6	0.565968	1.716560	-0.367345
6	1.764289	1.135528	0.374607
6	2.007751	-0.302199	-0.099407
8	0.802321	-1.069284	0.081372
8	-1.688936	1.411134	-1.026265
8	0.330234	3.022512	0.146907
8	2.944634	1.891029	0.127843
6	3.097680	-1.019792	0.687447
8	3.302594	-2.347134	0.219898
1	-2.565140	1.295346	-0.587969
1	-0.489256	3.344731	-0.267375
1	2.449220	-2.806371	0.277395
1	-0.976985	0.798471	0.830048
1	0.818857	1.785739	-1.438320
1	1.540582	1.124497	1.453404
1	2.279519	-0.296798	-1.166573
1	2.721909	2.827227	0.265894
1	2.835584	-1.016749	1.756916
1	4.044068	-0.490428	0.560075
8	-1.388579	-1.455436	-0.432737
1	-0.063764	-0.603821	-1.745660
6	-1.314797	-2.715679	-1.110818
1	-1.247790	-2.557159	-2.194449
1	-2.239486	-3.246734	-0.876569
1	-0.454261	-3.297402	-0.764726
8	-3.374778	-1.299813	1.508064
1	-3.083189	-1.356180	2.430080
1	-2.572741	-1.405738	0.949282
8	-4.044676	1.124040	0.400871
1	-4.882709	1.102789	-0.083933
1	-3.971292	0.261113	0.874589

D			
6	0.022228	1.046996	-0.336219
6	0.977129	-0.005774	0.256105
6	0.413723	-1.408440	-0.020808
6	-1.046746	-1.512870	0.427032
6	-1.883466	-0.394774	-0.197168
8	-1.295173	0.869973	0.162177
8	2.272658	0.093529	-0.333895
8	1.113923	-2.434327	0.665333
8	-1.597064	-2.763920	0.041891
6	-3.321692	-0.362960	0.303995
8	-4.069942	0.688469	-0.294537
1	2.751050	0.848471	0.077875
1	1.946188	-2.628769	0.178991
1	-3.607466	1.518867	-0.097681
1	1.037974	0.147883	1.342337
1	0.455487	-1.588301	-1.107267
1	-1.078735	-1.406610	1.523713
1	-1.887450	-0.496890	-1.293775
1	-0.939216	-3.438477	0.287130
1	-3.818188	-1.297089	0.033888
1	-3.322782	-0.270032	1.400980
8	0.451218	2.331341	0.034119
1	0.013595	0.965205	-1.437922
6	-0.199866	3.401583	-0.661317
1	-1.258990	3.451873	-0.391644
1	0.302475	4.321527	-0.355185
1	-0.096042	3.271420	-1.746364
8	3.091977	2.438206	0.897957
1	2.145760	2.662081	0.776883
1	3.282375	2.512455	1.844857
8	3.380399	-2.371636	-0.946358
1	3.243187	-1.404285	-0.837997
1	4.278944	-2.564973	-0.642033

E			
6	-0.498855	1.201856	-0.229462
6	-1.945318	0.707214	-0.137095
6	-1.975683	-0.670823	0.518155
6	-1.046123	-1.641074	-0.210445
6	0.354447	-1.024534	-0.312179
8	0.262766	0.242595	-0.980498
8	-2.755584	1.565165	0.662258
8	-3.280707	-1.247447	0.501017
8	-0.940362	-2.879597	0.481561
6	1.326965	-1.864081	-1.131213
8	2.576580	-1.175544	-1.291167
1	-2.721312	2.453584	0.270895
1	-3.888899	-0.619331	0.924743
1	2.355229	-0.290819	-1.632583
1	-2.347768	0.640549	-1.158288
1	-1.631645	-0.571017	1.559647
1	-1.439205	-1.805845	-1.226063
1	0.763276	-0.875376	0.698280
1	-1.843891	-3.181259	0.675288
1	0.900699	-2.083797	-2.119352
1	1.543533	-2.803596	-0.620473
8	-0.511590	2.416144	-0.903561
1	-0.035939	1.310173	0.763338
6	0.724258	3.141290	-0.867365
1	1.451797	2.697115	-1.556449
1	1.142067	3.150996	0.145994
1	0.491409	4.157679	-1.192854
8	2.102848	1.412016	2.005534
1	2.096794	1.423132	2.973826
1	2.789126	0.752200	1.755401
8	3.851285	-0.593232	1.114486
1	4.808233	-0.503150	0.998132
1	3.486463	-0.871124	0.241090

F			
6	-1.564905	0.810313	0.282839
6	-2.115648	-0.588281	-0.010596
6	-0.981607	-1.612065	0.044980
6	0.184156	-1.229419	-0.869357
6	0.634516	0.195898	-0.510601
8	-0.472951	1.100628	-0.608512
8	-3.112764	-0.888619	0.955779
8	-1.537688	-2.875965	-0.310233
8	1.233528	-2.185971	-0.778827
6	1.713194	0.734497	-1.435680
8	2.274847	1.959906	-0.932849
1	-3.339420	-1.827429	0.846255
1	-0.795945	-3.498010	-0.406579
1	1.540840	2.580613	-0.787222
1	-2.547739	-0.574265	-1.022164
1	-0.607326	-1.657166	1.081996
1	-0.156772	-1.254469	-1.911684
1	1.015792	0.198411	0.522937
1	1.743242	-2.039947	0.049849
1	1.298007	0.899049	-2.438028
1	2.540762	0.026529	-1.506498
8	-2.561987	1.741974	0.063477
1	-1.195750	0.866012	1.323350
6	-2.303156	3.040230	0.587620
1	-2.068845	2.988210	1.660751
1	-3.220326	3.615779	0.446359
1	-1.479516	3.531091	0.054932
8	2.727984	-1.440666	1.504440
1	3.097699	-1.948857	2.240695
1	3.234453	-0.594306	1.451735
8	3.871933	1.069727	1.163519
1	4.805212	1.213095	0.948262
1	3.353119	1.520510	0.455491

(c) Vibrational frequencies.

	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	38.4479	1.4168	28.0115	1.5182	31.3650	0.9761
v2	49.3835	2.2978	31.1626	1.2513	35.4780	0.8071
v3	61.4927	0.1778	44.7174	0.0831	44.9908	0.2320
v4	73.5670	0.3411	71.7227	5.2824	78.3710	3.5880
v5	84.5039	7.3078	84.0848	3.3888	80.8387	2.2524
v6	106.5362	0.5738	96.0602	4.4509	103.1306	6.9065
v7	114.3202	4.9886	112.3578	2.3004	117.0454	2.3935
v8	143.0445	2.7739	115.7736	4.9347	127.6487	1.1639
v9	165.7808	3.7778	143.4585	30.9014	145.7864	1.6236
v10	172.1915	26.6523	143.8185	29.6293	165.9745	18.1734
v11	179.5719	6.1762	168.8743	27.2614	173.5769	43.1459
v12	202.9977	57.9550	198.7116	55.6611	184.6880	14.6113
v13	204.9610	95.8303	208.4637	3.0478	189.9317	1.8953
v14	221.6113	4.8040	223.2776	1.5603	228.5392	43.0401
v15	250.8121	2.5277	248.2505	5.4754	233.7107	22.6570
v16	257.9481	1.9548	253.9105	25.3503	249.5644	42.3714
v17	269.5516	37.7249	259.4135	23.7597	260.8705	24.7617
v18	278.7211	47.5185	275.2017	11.6664	278.3982	34.4819
v19	284.4707	4.1753	286.1643	2.0225	281.4641	13.4014
v20	317.1299	11.5248	313.8127	37.7062	295.0443	13.6259
v21	331.7280	21.9481	329.2479	9.3115	317.1902	4.3463
v22	336.9892	3.9874	337.5189	18.4585	364.7423	7.1521
v23	346.0565	34.8076	370.8595	47.6526	368.1785	45.9103
v24	389.0418	84.5266	389.6622	87.5422	393.3291	10.2081
v25	414.1287	10.5731	406.7521	34.7084	400.9054	15.4239
v26	421.7914	11.7460	425.3515	20.4939	413.2656	232.6252
v27	439.2299	82.1639	431.1827	59.0600	423.7089	5.3303
v28	453.6345	30.3058	457.2792	23.4751	442.9822	98.1192
v29	463.3086	65.6036	469.0005	131.5266	467.4664	9.1002
v30	531.0324	17.3943	523.0492	5.8385	495.9045	3.5811
v31	556.6402	45.5312	546.2075	62.7095	528.9063	74.2764
v32	573.9267	3.7251	570.9141	6.3371	585.5362	15.1558
v33	608.6248	22.3834	608.8883	17.6529	617.8479	8.4466
v34	613.5799	20.5813	617.8984	3.9278	627.1697	19.3185
v35	716.4124	0.4814	630.2437	77.5102	641.3075	37.7375
v36	748.1496	39.9192	718.7847	1.0192	643.0935	18.5589
v37	777.8829	229.0132	762.7663	113.5133	764.4812	142.6963
v38	890.6715	24.3676	916.5176	7.1523	889.8003	28.4510
v39	923.7008	7.4753	919.3743	49.2009	985.5937	31.3156
v40	987.2439	11.3033	989.5067	9.4358	1009.1773	24.7853
v41	1020.3813	328.7082	1023.8338	316.7904	1033.4290	65.1253
v42	1027.3584	98.3056	1026.9652	48.7162	1051.5362	46.0417
v43	1051.0647	84.0543	1046.1627	79.6542	1061.2027	300.8232
v44	1072.2179	82.9562	1072.0040	13.9796	1076.8815	51.0496
v45	1083.6033	30.5334	1076.4204	179.4118	1085.1727	7.6539
v46	1096.2748	37.6438	1098.6354	37.9074	1093.0821	256.3910
v47	1114.9303	94.9763	1115.3386	116.0086	1109.5253	27.9301
v48	1135.0752	92.0352	1125.1927	55.1713	1121.7257	19.8107
v49	1137.4057	10.6464	1134.9409	18.0451	1129.4390	153.2629
v50	1147.9636	25.1708	1143.9178	44.2858	1146.4161	8.6284
v51	1176.0287	55.7151	1177.9081	59.7139	1170.1100	38.8105
v52	1183.3940	13.1408	1181.6975	4.7119	1179.3061	5.7885
v53	1213.7481	70.9520	1217.2913	78.4186	1209.8988	8.5889
v54	1224.5134	27.4310	1235.8216	1.4353	1230.5934	28.8811
v55	1229.6771	42.0023	1237.5495	46.6319	1237.4921	88.1289
v56	1245.6253	16.0385	1252.9319	27.6714	1240.0187	9.6168
v57	1265.5280	43.4984	1254.6667	34.6746	1244.4581	25.4776
v58	1271.6969	21.0210	1266.8940	50.1380	1264.8186	29.6115
v59	1287.0031	29.1215	1277.2840	25.4360	1282.4704	10.8328
v60	1317.6067	25.6337	1314.3339	34.3601	1314.8325	11.0209
v61	1335.5413	6.8544	1326.7481	9.7706	1325.0663	52.3534
v62	1351.4270	42.9458	1353.0612	31.2403	1348.2376	0.5511
v63	1368.9900	31.3237	1363.8219	19.6541	1362.3817	29.7859
v64	1393.6502	0.2965	1367.7923	18.5736	1379.5194	14.9784
v65	1398.9396	22.9596	1396.9280	31.8241	1401.9447	1.8469
v66	1410.2146	19.4616	1410.7442	7.5548	1405.7233	29.1145
v67	1421.3824	7.0572	1422.1299	9.5021	1429.8914	22.0467
v68	1438.2525	2.5495	1438.6072	24.9175	1432.8173	39.9850
v69	1459.7002	33.0995	1441.5976	26.8672	1441.7474	2.2524
v70	1484.9029	16.6515	1460.6522	32.2076	1451.1966	18.8247
v71	1493.2835	32.6221	1490.9752	19.1205	1493.6623	7.8154
v72	1497.7723	5.0431	1497.8606	6.8112	1495.6665	18.3369
v73	1510.2927	1.5342	1508.6474	6.3073	1508.9438	8.9804
v74	1511.4553	28.7683	1521.5468	6.3909	1517.3270	2.2523
v75	1526.2098	6.5461	1527.3886	6.5696	1526.5693	8.0467

v76	2514.2076	258.4667	2491.9957	298.4827	2505.1944	257.0481
v77	2596.4030	162.9624	2532.4171	365.2183	2568.6634	300.0965
v78	2790.3221	80.0888	2787.6509	62.5890	2786.0024	73.0566
v79	2792.4304	91.0718	2793.6965	89.3602	2786.9354	84.1477
v80	2984.0891	6.7593	2968.5552	25.5486	2983.7220	16.7061
v81	2989.0333	8.9298	2987.9907	17.5330	2995.1676	15.1144
v82	2998.2525	49.8037	3003.1735	32.1657	3004.8878	9.7352
v83	3025.6210	37.1020	3024.7486	58.2801	3010.8101	9.0878
v84	3031.6010	62.6908	3030.6244	35.2838	3026.5318	62.2122
v85	3049.8803	45.9568	3052.6819	38.5996	3038.1339	78.5749
v86	3060.5549	36.8631	3054.8082	57.9496	3045.1384	53.9669
v87	3096.8750	32.3132	3091.5682	37.9882	3116.9865	26.9439
v88	3123.3388	23.3246	3138.1912	14.0294	3147.0325	9.9374
v89	3158.7582	20.5650	3154.6981	23.7419	3161.5737	15.1727
v90	3458.2351	559.6758	3452.4452	933.0210	3446.7464	924.7846
v91	3495.6722	633.2005	3697.7077	70.6984	3714.3483	52.5832
v92	3715.5545	53.0992	3720.3121	48.4537	3727.4188	52.5487
v93	3727.4981	51.4174	3727.0115	50.2747	3743.3978	24.7866

	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
v1	37.1697	3.2816	22.2379	1.6151	30.7065	6.8859
v2	39.4693	0.3915	35.6598	0.4954	38.5258	7.3114
v3	61.9149	1.0861	40.3845	1.1441	47.3752	0.6399
v4	78.8168	2.6276	62.8629	1.5881	59.2246	45.3958
v5	96.9169	6.1505	81.3502	7.9889	75.6147	7.7338
v6	104.3239	0.5759	87.7325	0.7530	89.8190	3.2937
v7	121.0377	1.9806	108.0222	3.5652	101.3519	8.3110
v8	132.1503	5.7970	117.2931	8.9898	109.6879	2.5308
v9	138.5811	4.9189	128.8258	30.4676	128.7112	0.5825
v10	162.0271	10.0556	136.2769	39.7230	149.9658	1.6579
v11	171.4773	0.3447	142.7970	1.8996	169.2858	36.0608
v12	180.3726	7.7021	154.9903	44.5948	183.2732	32.4477
v13	190.2876	14.6144	182.3136	1.2141	210.5825	4.4539
v14	204.6812	79.0844	219.4073	22.7697	219.1033	9.1359
v15	222.1647	87.4831	225.3877	3.3899	231.9915	3.7423
v16	235.6738	21.9619	232.4250	24.4924	251.5128	3.9044
v17	250.1433	11.7168	243.1981	19.1083	256.4458	16.8655
v18	266.5175	18.6400	256.2407	12.8895	266.9329	39.7901
v19	294.5719	33.0370	279.9586	44.6336	285.6603	11.6324
v20	315.3288	18.2658	294.9278	6.6163	305.4834	6.8896
v21	335.1654	6.8220	306.7288	5.2247	315.4013	12.5719
v22	350.2888	7.6808	336.4488	31.9614	365.2428	58.6722
v23	376.2727	18.7402	365.7170	11.6618	368.1840	18.0750
v24	395.0310	16.3404	376.8199	78.6611	384.5195	99.6048
v25	402.5802	93.5238	396.1283	71.3148	389.4684	20.2041
v26	424.4004	0.8561	401.5109	48.7653	416.6059	36.4163
v27	450.9240	200.0847	407.6405	144.0373	425.9279	44.1775
v28	463.7112	19.0838	422.4058	4.0617	455.0129	71.3100
v29	477.9533	15.3627	452.9403	85.9228	457.5790	9.2332
v30	498.4941	4.7994	462.1890	29.1843	504.4988	18.0121
v31	507.9995	121.8764	495.3719	14.7344	538.0073	84.4301
v32	587.0100	20.4411	546.9310	128.4379	582.7893	13.5889
v33	620.4518	9.9917	587.0642	14.5185	601.1672	71.8740
v34	630.5542	30.6687	610.4840	6.0814	614.8956	12.5924
v35	639.8792	11.1590	620.5813	12.4619	629.3255	9.0647
v36	771.1204	106.1110	642.2114	24.1585	640.7000	13.3543
v37	788.8966	116.9785	652.3059	111.2119	750.8510	141.5541
v38	892.0799	28.1405	898.2543	28.0208	891.5952	37.9865
v39	978.4724	16.1810	973.6509	16.9934	989.8575	11.3980
v40	1013.9366	43.9972	1000.8067	44.9671	1003.5857	134.4405
v41	1036.6750	8.1654	1020.8350	103.4427	1010.0024	136.4977
v42	1054.7129	138.2891	1043.4280	191.0029	1035.9708	191.2358
v43	1067.4690	217.9511	1053.4669	45.0242	1049.6003	4.8244
v44	1073.1857	47.6724	1067.5123	21.3109	1076.3747	102.3496
v45	1084.2960	19.8856	1087.3185	171.9965	1080.9302	23.1413
v46	1095.0238	214.2280	1088.6046	93.0265	1090.1979	101.6962
v47	1109.5036	56.1171	1107.4505	40.3983	1112.1253	65.1201
v48	1119.7310	192.1747	1116.1552	157.1047	1124.4144	127.9192
v49	1127.9408	25.1796	1122.6618	52.0870	1137.9302	44.3840
v50	1146.0469	3.3469	1148.4245	7.0434	1152.4349	5.4524
v51	1170.7834	25.9183	1178.2756	32.5664	1179.0968	9.2756
v52	1178.3074	2.7268	1185.2754	19.1439	1180.7849	39.8159
v53	1215.3264	2.9752	1208.6228	13.2612	1213.2209	10.1319
v54	1219.6477	48.1151	1233.8067	23.7670	1232.5145	96.7810
v55	1230.3968	50.5250	1242.2212	79.2907	1243.4624	29.2728
v56	1233.6304	50.2835	1243.3488	11.7670	1248.6136	36.6512
v57	1246.1993	0.8851	1253.7064	40.9270	1253.1655	36.5638
v58	1273.6544	24.6721	1258.0102	40.6915	1262.0086	10.4691
v59	1292.6203	31.1094	1267.3731	40.4138	1269.7722	56.0752
v60	1316.5029	9.6744	1316.8463	21.9214	1301.2774	33.1233
v61	1334.7421	31.9552	1335.8691	34.1435	1338.0676	6.0000
v62	1350.1823	5.7216	1352.0420	46.4847	1345.5317	43.5121
v63	1379.1666	18.6913	1354.8546	12.3939	1358.8731	7.8109
v64	1396.8081	11.3643	1375.0050	3.3798	1381.7293	35.1344
v65	1400.9468	25.2342	1386.3771	14.1724	1397.4688	22.9696
v66	1408.3224	40.1973	1414.0221	7.8063	1413.7769	1.9940
v67	1429.0649	16.8235	1428.1436	10.5209	1420.1027	4.0362
v68	1434.0636	34.2553	1437.8664	18.7061	1437.6061	3.2556
v69	1453.3912	17.7874	1440.4432	2.7110	1446.1373	35.4220
v70	1469.8832	35.3803	1450.5589	34.1095	1460.5235	29.4115
v71	1488.8694	11.1508	1460.2920	17.6166	1467.8196	46.2844
v72	1493.3373	6.5548	1503.1224	8.0974	1497.4547	6.1169
v73	1504.3861	8.3163	1507.8985	7.5797	1507.8150	6.6478
v74	1516.4710	2.6847	1518.5619	2.4162	1517.6033	4.9934
v75	1527.2229	9.4856	1533.6165	9.7916	1526.8328	7.1191

v76	2565.0377	200.1507	2510.5334	314.2717	2490.9188	281.4212
v77	2602.5134	137.3540	2554.8132	248.1651	2530.8879	314.3032
v78	2792.4821	47.6317	2783.3595	53.0699	2784.2718	78.1656
v79	2793.0023	137.7974	2787.5210	79.9717	2792.0909	64.0081
v80	2973.4340	28.1684	3004.9556	3.9699	2964.3260	28.0586
v81	2995.3755	4.4696	3014.3405	16.7442	2987.1635	24.1264
v82	3006.2379	10.7529	3026.4405	5.2292	3012.6553	13.8959
v83	3013.0405	5.8611	3032.3130	6.9657	3021.4880	60.1891
v84	3026.7458	89.4544	3044.1577	41.7896	3033.6991	32.0478
v85	3042.7151	47.0594	3045.7238	35.7673	3061.5796	10.2153
v86	3050.7024	48.8653	3051.6771	84.3219	3072.0869	64.3110
v87	3120.2004	27.7918	3113.8864	24.8702	3085.6387	43.7885
v88	3147.4464	9.5644	3151.7478	25.1490	3152.7339	25.9090
v89	3158.8555	18.1719	3158.7353	8.3622	3155.8762	9.1264
v90	3497.3385	623.8685	3707.5295	50.4910	3518.3987	443.5415
v91	3508.4514	650.7303	3727.9812	49.4563	3716.8680	47.6434
v92	3704.4791	53.9708	3738.3353	44.9863	3729.8069	47.8969
v93	3744.4915	24.2359	3740.6790	54.8010	3731.7841	44.6858

The experimental R2PI spectra of various molecules of interest are given below.

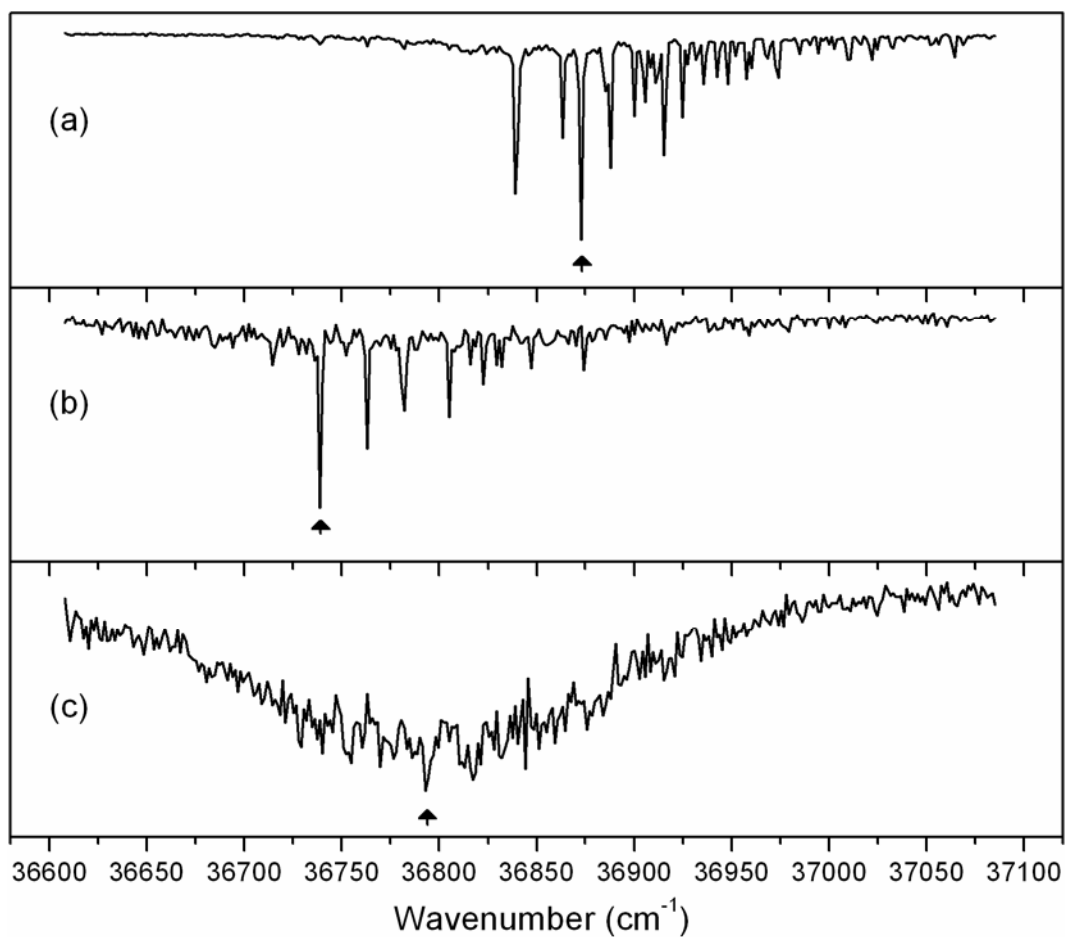


Figure S1. R2PI spectra (a,b,c) of $\alpha\text{-PhGlc}\cdot(\text{D}_2\text{O})_{0,1,2}$. The arrows indicate bands selected in recording the complementary IRID spectra.

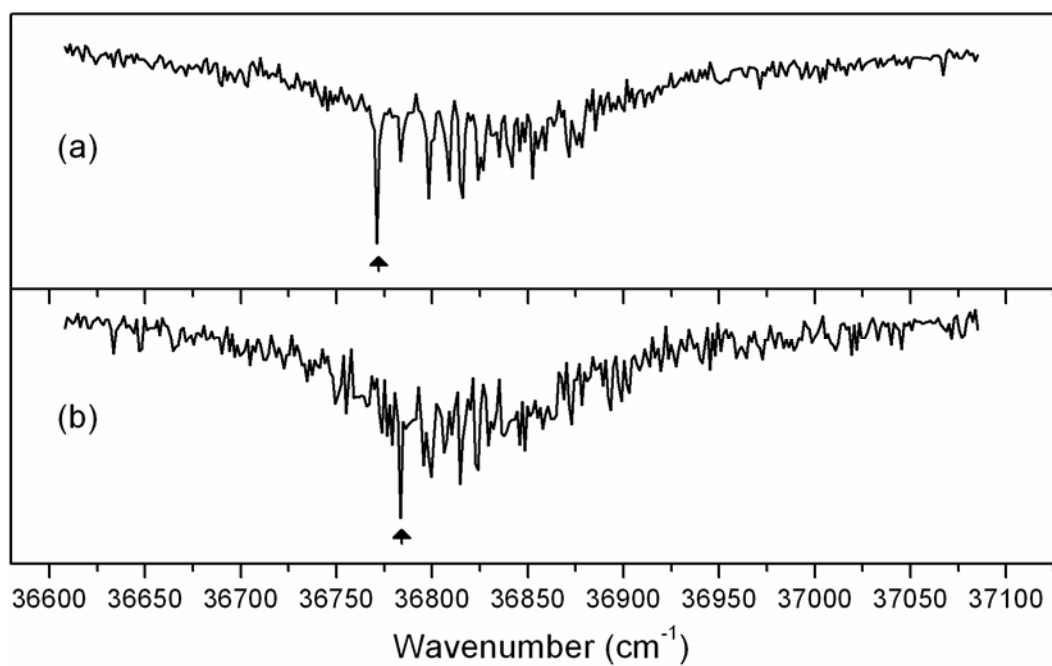


Figure S2. R2PI spectra (a,b) of β -PhGlc $\cdot$ (D₂O)_{1,2}. The arrows indicate bands selected in recording the complementary IRID spectra.

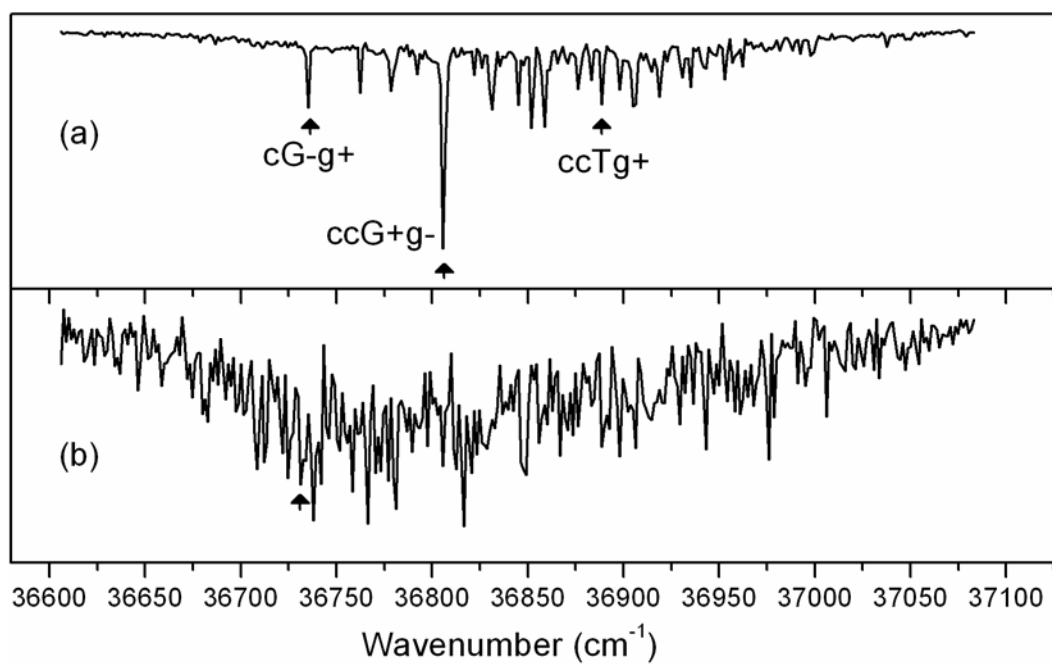


Figure S3. R2PI spectra (a,b) of α -PhGal $\cdot$ (D₂O)_{0,1}. The arrows indicate bands selected in recording the complementary IRID spectra.

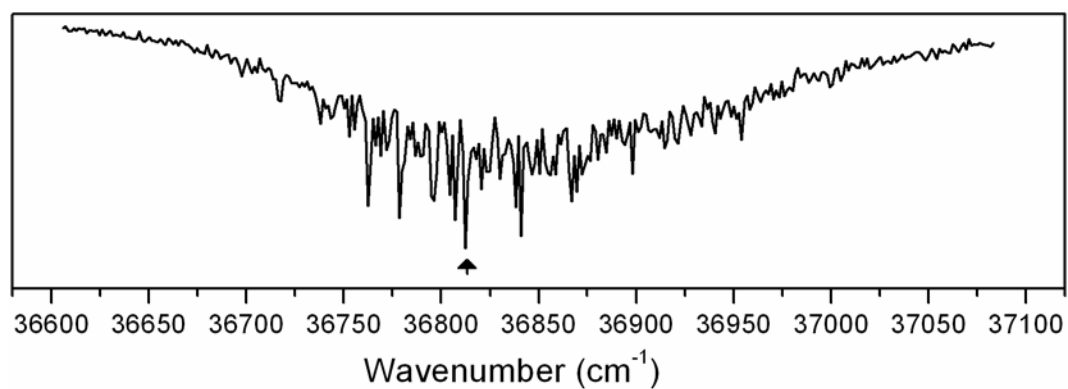


Figure S4. R2PI spectrum of β -PhGal·D₂O. The arrow indicates band selected in recording the complementary IRID spectrum.

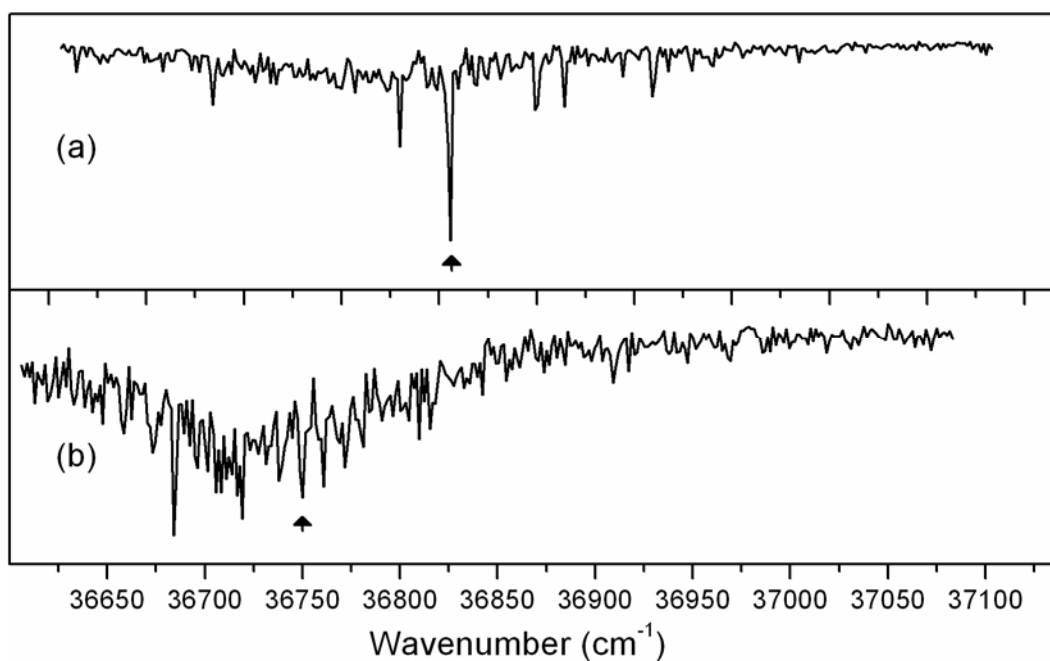


Figure S5. R2PI spectra (a,b) of α -PhFuc $\cdot$ (D₂O)_{1,2}. The arrows indicate bands selected in recording the complementary IRID spectra.

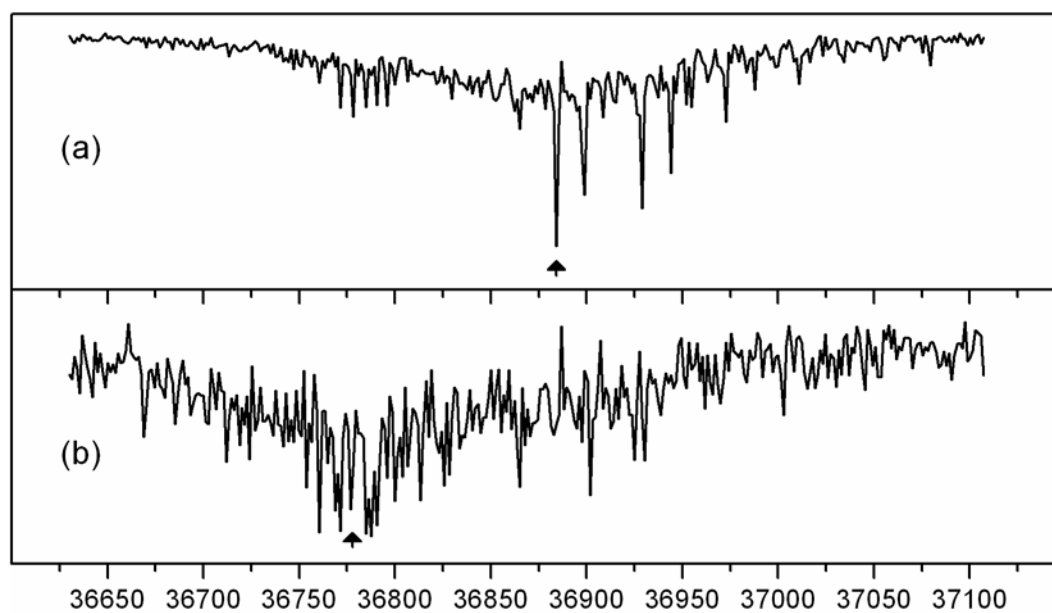


Figure S6. R2PI spectra (a,b) of α -PhXyl·(D₂O)_{1,2}. The arrows indicate bands selected in recording the complementary IRID spectra.

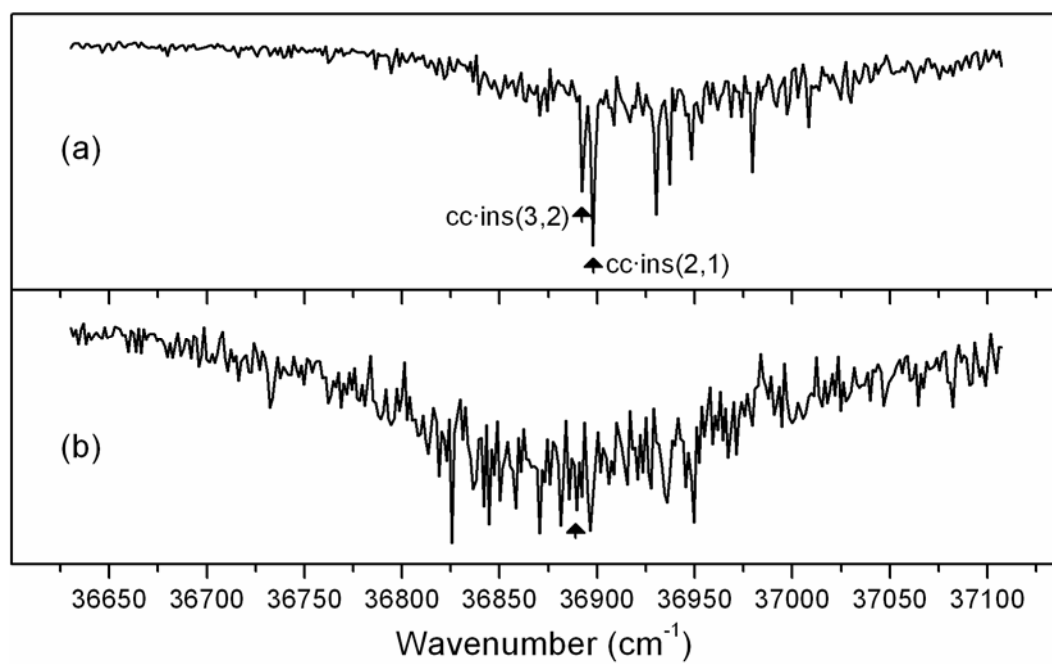


Figure S7. R2PI spectra (a,b) of β -PhXyl $\cdot$ (D₂O)_{1,2}. The arrows indicate bands selected in recording the complementary IRID spectra.