Heavy water hydration of mannose: the anomeric effect in solvation, laid bare

Nitzan Mayorkas,[a] Svemir Rudić,[b,c] Benjamin G. Davis[c,*] and John P. Simons[b,*]

[a] *Department of Physics, Ben-Gurion University of the Negev, Beer Sheva 84105, Israel.*

[b] *Department of Chemistry, University of Oxford, Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ, UK. Fax: +44 (0)1865 275410, Tel: +44 (0)1865 275400, E-mail: john.simons@chem.ox.ac.uk*

[c] *Department of Chemistry, University of Oxford, Chemistry Research Laboratory, Mansfield Road, Oxford OX1 3TA, UK. Fax: +44 (0)1865 285002, Tel: +44 (0)1865 275652, E-mail: ben.davis@chem.ox.ac.uk*

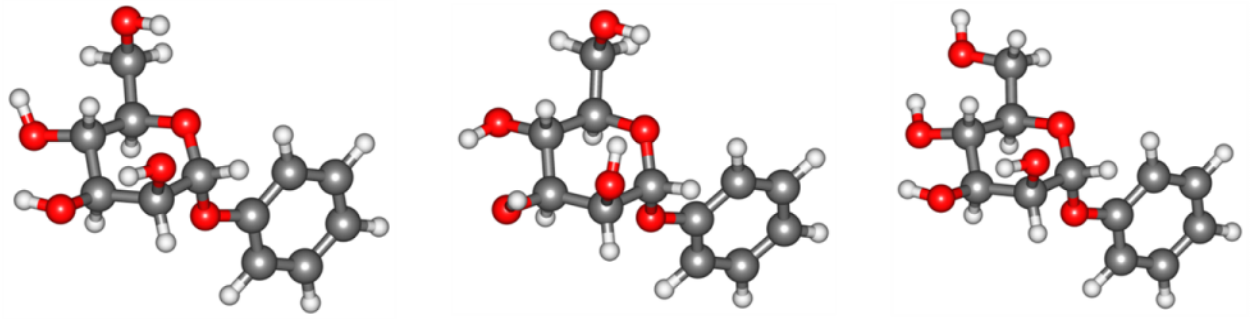
Supplementary information

The relative energies, Cartesian coordinates of optimized geometries, and the vibrational frequencies of the low energy conformers of α- and β-Phenyl mannopyranoside•$(D_2O)_{0-3}$, are given in this supplementary information. They were obtained using the Gaussian 03 package of programs, and derived at the B3LYP/6-311++G(d,p) [α- and β-PhMan•$(D_2O)_{0,1,2}$] and B3LYP/6-31+G(d) [α- and β-PhMan•$(D_2O)_3$] levels of theory. More accurate relative 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. In the tables listing the atomic coordinates (in the optimized geometries), the first column indicates the atomic number, and the subsequent columns provide the *x*, *y* and *z* coordinates, respectively. When present, coordinates of the D_2O molecule(s) are given at the foot of the tables. The origin of each coordinate system is its molecular centre-of-mass. The geometrical coordinates are taken from the 'standard orientation' table of the output file for each calculation. Comparisons between experimental IRID spectra of α-PhMan•$(D_2O)_{2 \text{ and } 3}$ and the calculated vibrational (stick) spectra of each of the relatively low energy structures associated with the corresponding complex are also provided in Figures S1 and S2.

1. α-PhMan

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

Conformer	B3LYP/6-311++G(d,p) energy / kJ mol^{-1}	MP2/6-311++G(d,p)//B3LYP/6-311++G(d,p) energy / kJ mol^{-1}
A	0.00	0.00
B	3.70	3.04
C	1.61	3.47



A B C

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

A			
6	0.036030	-0.523503	0.828916
6	-1.092389	-1.560177	0.772188
6	-1.995370	-1.315526	-0.439683
6	-2.439603	0.141375	-0.491410
6	-1.205180	1.054176	-0.507569
8	-0.421984	0.800161	0.676059
8	-1.820160	-1.446563	1.985876
8	-3.108364	-2.197866	-0.309521
8	-3.232551	0.288852	-1.675823
6	-1.533135	2.540532	-0.476540
8	-2.380304	2.897804	0.608414
1	-2.638781	-1.944843	1.865457
1	-3.753914	-1.944816	-0.980417
1	-1.935969	2.638328	1.424184
1	0.509170	-0.554105	1.812562
1	-0.637242	-2.553536	0.688719
1	-1.436622	-1.547443	-1.355143
1	-3.037196	0.368645	0.394829
1	-0.607098	0.845405	-1.403331
1	-3.841789	1.023484	-1.552360
1	-2.061581	2.820016	-1.390166
1	-0.592573	3.103493	-0.446186
8	0.958743	-0.888119	-0.184082
6	4.929705	0.382254	-0.157833
6	4.489871	-0.640084	-1.000681
6	3.159240	-1.041285	-0.986973
6	2.253359	-0.415497	-0.126669
6	2.676744	0.617713	0.711143
6	4.018989	1.002431	0.691850
1	5.968065	0.691661	-0.167536
1	5.187490	-1.132767	-1.668675
1	2.804614	-1.840040	-1.627294
1	1.975576	1.134148	1.352035
1	4.345256	1.803771	1.345511

B			
6	0.016762	-0.484713	0.890831
6	-1.137403	-1.493198	0.892050
6	-1.965313	-1.354999	-0.390773
6	-2.396377	0.098298	-0.616365
6	-1.191885	1.041859	-0.543427
8	-0.474858	0.828161	0.697244
8	-1.955918	-1.307254	2.049266
8	-3.100890	-2.215216	-0.373645
8	-2.985219	0.258233	-1.900303
6	-1.572549	2.517429	-0.559385
8	-2.343665	2.895928	0.575205
1	-2.126854	-0.363151	2.157192
1	-3.467240	-2.186971	0.520823
1	-1.783575	2.793065	1.352106
1	0.508949	-0.467582	1.866686
1	-0.737907	-2.504979	0.971012
1	-1.357533	-1.669652	-1.242774
1	-3.116211	0.392997	0.160131
1	-0.528049	0.836714	-1.390362
1	-3.658588	-0.426595	-1.994191
1	-2.187563	2.711925	-1.438222
1	-0.659394	3.120689	-0.629208
8	0.918667	-0.888826	-0.115720
6	4.898746	0.352307	-0.182554
6	3.989984	1.048866	0.607963
6	2.645630	0.673822	0.655891
6	2.221044	-0.425207	-0.091354
6	3.123390	-1.128647	-0.891802
6	4.456188	-0.736486	-0.935885
1	5.938669	0.654542	-0.216216
1	4.319193	1.902333	1.190112
1	1.943397	1.246888	1.245622
1	2.765498	-1.976714	-1.463032
1	5.152981	-1.287693	-1.557193

C			
6	0.083415	-0.797299	0.784655
6	-1.046876	-1.788998	0.484622
6	-1.979258	-1.225431	-0.585992
6	-2.435313	0.188531	-0.242507
6	-1.213130	1.083861	0.020503
8	-0.382523	0.506781	1.038467
8	-1.734156	-2.021440	1.704817
8	-3.090327	-2.116919	-0.680340
8	-3.213467	0.629185	-1.352517
6	-1.579056	2.456900	0.576541
8	-2.459861	3.099239	-0.357022
1	-2.564581	-2.457263	1.473851
1	-3.752764	-1.693275	-1.239646
1	-2.714440	3.960785	-0.014495
1	0.602966	-1.097136	1.697090
1	-0.594461	-2.716951	0.116303
1	-1.443384	-1.190110	-1.541988
1	-3.047878	0.154352	0.668296
1	-0.647797	1.201544	-0.911674
1	-3.374431	1.577418	-1.244518
1	-0.664833	3.042351	0.716379
1	-2.068390	2.326893	1.548459
8	0.957645	-0.847277	-0.331439
6	4.901257	0.493248	-0.161597
6	4.036944	0.811558	0.881414
6	2.704887	0.392616	0.865129
6	2.244873	-0.368857	-0.210977
6	3.104355	-0.690420	-1.265028
6	4.424871	-0.258276	-1.237420
1	5.931737	0.827560	-0.140520
1	4.391946	1.401371	1.719306
1	2.038159	0.677886	1.667018
1	2.721717	-1.282108	-2.087985
1	5.086112	-0.514470	-2.057668

(c) Vibrational frequencies.

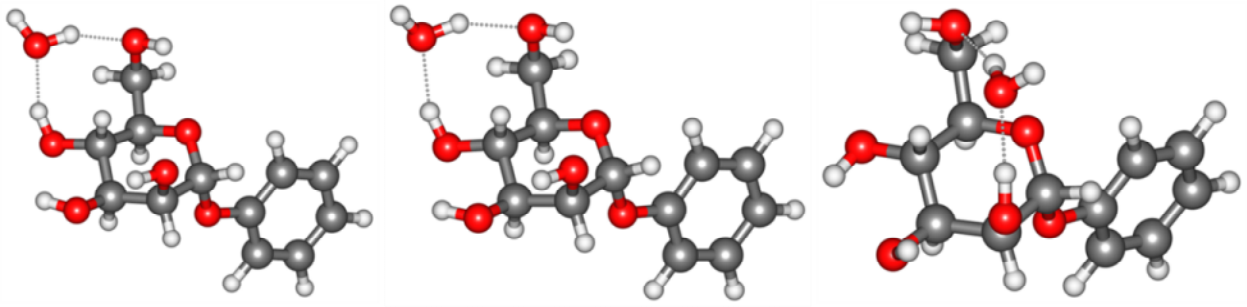
	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
ν1	30.1094	0.0539	29.2023	0.1077	27.8774	0.3101
ν2	44.0540	0.1215	44.0650	0.0325	46.7140	0.0824
ν3	50.0598	0.2889	49.4570	0.7206	50.9691	1.0092
ν4	76.2236	5.0522	90.5984	2.1573	81.4860	0.5633
ν5	104.8381	0.6073	100.3349	4.1980	104.5458	1.4767
ν6	113.5547	2.7769	120.9623	2.3117	134.3136	6.9419
ν7	144.8364	4.7109	146.5600	0.4538	151.0774	6.3876
ν8	196.1884	3.3297	195.3559	5.5843	202.2778	3.9697
ν9	209.7037	3.3402	204.9194	1.4412	208.4074	7.5634
ν10	247.8718	9.7128	243.3779	3.6290	234.2269	6.0336
ν11	258.5542	9.9735	253.3682	4.3755	254.2026	2.5487
ν12	262.6347	10.9120	260.9876	9.0676	258.7248	81.2836
ν13	273.8868	7.3911	270.4124	20.3470	276.2814	1.9643
ν14	327.7453	4.9347	323.2294	3.8286	301.8701	3.7715
ν15	341.4668	70.1035	352.7521	19.8686	352.2420	11.0054
ν16	366.5534	6.4617	370.4437	30.6590	363.2468	9.3544
ν17	394.0079	18.3034	392.5591	95.7418	382.0311	9.7799
ν18	417.2783	203.7012	408.5402	75.2590	418.4045	49.8604
ν19	421.2501	1.7457	413.1213	44.3476	420.9961	4.7511
ν20	429.0941	53.8013	420.7629	0.0500	424.4806	129.2514
ν21	439.3475	63.6783	442.4532	12.4502	447.5571	15.8614
ν22	451.9834	41.1075	480.8939	2.5662	466.0317	31.6188
ν23	485.7646	13.4643	504.0704	19.9665	507.5245	46.2056
ν24	508.5900	23.0603	512.6919	193.6726	517.7713	12.5336
ν25	521.4103	4.5440	519.8244	2.0671	535.8683	68.1935
ν26	580.3985	9.4175	579.4329	6.2146	543.6076	36.0778
ν27	619.0818	9.2693	618.7366	4.0950	583.6735	1.6539
ν28	639.7439	23.8180	638.4683	7.6710	623.4117	2.7558
ν29	678.2482	4.7634	665.9147	1.9816	661.2425	45.6429
ν30	686.8097	37.0845	686.9571	23.8216	683.8129	17.2924
ν31	701.5545	25.3886	701.7852	22.2289	701.3817	24.6787
ν32	765.6405	64.1328	766.3033	66.9224	765.6903	65.9102
ν33	806.7704	22.7707	804.1337	16.2673	801.6043	17.6163
ν34	834.4022	1.6385	834.8608	1.4223	834.2433	1.1997
ν35	842.1456	10.3292	844.8086	12.3271	846.0318	23.5671
ν36	851.9084	20.4531	857.3186	34.7814	878.1083	14.2387
ν37	883.8466	11.7139	873.8657	54.3624	904.1884	3.3465
ν38	904.6286	5.2811	906.2668	4.3238	915.2241	12.9733
ν39	926.1245	10.2052	915.5597	22.9835	949.3708	6.3047
ν40	973.6969	2.9551	974.3640	12.6406	973.5271	0.0387
ν41	984.7882	151.4583	978.0185	52.3868	989.0126	0.0228
ν42	989.9141	8.4461	991.8555	0.6006	1007.9095	252.1426
ν43	1010.1319	147.2483	1008.4643	229.4910	1011.1119	38.7523
ν44	1018.5906	217.7505	1014.3168	16.4518	1019.7067	179.4396
ν45	1037.4458	40.8129	1032.7269	25.2279	1041.0427	25.0292
ν46	1044.7410	49.8642	1042.5359	13.7610	1050.4916	26.7387
ν47	1050.5708	92.0740	1059.6520	182.3958	1051.8507	126.6138
ν48	1072.7414	95.2253	1082.1681	46.5642	1083.4059	150.1913
ν49	1089.3728	69.8661	1090.4890	166.9718	1098.3099	17.2673
ν50	1103.5530	27.4958	1096.2745	131.7905	1103.3277	17.4929
ν51	1106.4351	14.3232	1101.2594	35.2049	1113.6682	77.5368
ν52	1118.3530	89.3034	1112.8320	25.8954	1117.9335	36.6880
ν53	1122.4643	58.8179	1119.2159	55.1026	1132.1560	106.5707
ν54	1131.9333	28.5435	1149.0736	20.2109	1141.5678	18.8490
ν55	1178.7851	3.8291	1179.7207	5.2946	1178.7982	3.1898
ν56	1197.3735	16.9272	1195.7093	26.0212	1196.6256	15.5834
ν57	1211.6403	79.8619	1216.9721	43.3677	1221.5769	46.9935
ν58	1223.8348	22.9423	1224.4041	183.9811	1242.4294	110.2754
ν59	1246.7711	233.7460	1242.4371	36.5767	1243.0731	42.4630
ν60	1252.1096	39.7312	1246.8392	124.3120	1250.1302	164.3422
ν61	1260.9015	29.3897	1271.8540	66.9321	1256.9976	45.8316
ν62	1269.8159	10.0448	1302.7859	2.0188	1277.0315	6.6766
ν63	1323.6845	3.1422	1320.6410	7.6790	1317.7890	3.7703
ν64	1341.6104	4.7537	1332.0322	8.8639	1322.7393	5.2428
ν65	1342.7149	10.1270	1343.6643	1.2502	1341.6075	8.0045
ν66	1355.5484	6.3124	1348.2009	3.0288	1346.2561	23.3308
ν67	1364.8510	12.8984	1354.8231	2.8724	1355.7571	6.3721
ν68	1369.5188	29.2554	1363.3733	39.4441	1360.2959	39.2723
ν69	1385.2959	11.4636	1385.4190	10.8002	1379.5079	16.6606
ν70	1395.9706	21.7001	1397.1946	25.8185	1397.1416	14.7708
ν71	1412.1333	35.1440	1413.6805	6.5274	1418.2353	34.7344
ν72	1415.7796	8.8289	1416.2452	17.9844	1421.0666	23.5480
ν73	1426.2979	10.9948	1424.5274	26.0912	1429.7217	2.6656

v74	1433.9437	6.7526	1429.0085	35.8274	1440.3527	15.9158
v75	1439.3547	34.6829	1439.2661	7.2175	1461.4773	9.0962
v76	1486.8240	1.4420	1486.9567	0.8462	1486.5416	1.2427
v77	1500.1137	7.0120	1494.2344	8.0423	1519.8509	4.6346
v78	1522.4836	109.8578	1522.0185	105.7839	1522.4937	111.4450
v79	1626.7889	26.3857	1627.7349	26.6089	1626.0560	25.6387
v80	1640.0119	65.9542	1640.0131	58.3620	1640.0302	68.1043
v81	3015.1342	23.3882	2992.5065	22.6367	3002.9413	7.1203
v82	3017.2848	1.5413	3015.5857	35.1885	3015.2892	26.8403
v83	3028.5375	31.5380	3046.9550	26.5784	3022.9689	11.3077
v84	3032.6130	50.3663	3068.7816	15.0684	3029.6826	19.8663
v85	3075.9308	14.9678	3077.2986	17.0344	3036.5641	53.9832
v86	3085.0138	17.0574	3100.3015	16.5121	3065.7880	41.2669
v87	3093.5286	21.0155	3118.3505	7.4796	3083.8605	16.7361
v88	3165.6533	1.0551	3167.0008	1.0415	3164.9970	1.1489
v99	3173.6500	10.9544	3175.0146	9.9905	3172.9501	11.7550
v90	3187.8004	19.8444	3188.9089	18.0051	3187.6558	20.6830
v91	3195.2978	7.3630	3196.5429	6.4727	3195.3223	6.9550
v92	3213.6846	1.1723	3210.7636	1.1213	3211.8983	0.9871
v93	3791.5533	77.6612	3770.4865	53.4702	3744.2121	189.4852
v94	3809.2266	61.8027	3792.9529	33.3431	3790.8443	77.2539
v95	3811.7773	36.1995	3803.9984	62.0291	3808.7777	63.2200
v96	3842.8191	56.6722	3826.2754	27.9969	3856.0815	57.2988

2. α-PhMan•$(D_2O)_1$

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

Conformer	B3LYP/6-311++G(d,p) energy / kJ mol^{-1}	MP2/6-311++G(d,p)//B3LYP/6-311++G(d,p) energy / kJ mol^{-1}
A	0.00	0.00
B	0.34	0.22
C	8.02	5.58



A B C

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

A			
6	-0.456171	0.686216	0.825488
6	0.544155	1.845867	0.733741
6	1.491114	1.658234	-0.454726
6	2.109747	0.263742	-0.436117
6	0.978978	-0.778357	-0.444157
8	0.154338	-0.582236	0.723800
8	1.259818	1.871791	1.960194
8	2.492582	2.667173	-0.350982
8	2.963271	0.149810	-1.567436
6	1.444220	-2.223323	-0.384049
8	2.281178	-2.495177	0.748785
1	2.030253	2.436801	1.815555
1	3.197214	2.422826	-0.964750
1	1.820649	-2.187995	1.539715
1	-0.938382	0.696422	1.805263
1	-0.024775	2.773437	0.602997
1	0.927060	1.783763	-1.387742
1	2.686488	0.151697	0.486502
1	0.375945	-0.655444	-1.352453
1	3.710863	-0.421665	-1.316269
1	2.037957	-2.455352	-1.268339
1	0.568936	-2.880690	-0.367203
8	-1.406064	0.900290	-0.204587
6	-5.181046	-0.868728	-0.192011
6	-4.216336	-1.336113	0.695130
6	-2.934891	-0.781584	0.721568
6	-2.629392	0.267006	-0.148001
6	-3.590286	0.740215	-1.045650
6	-4.858107	0.171302	-1.065544
1	-6.170838	-1.309320	-0.206912
1	-4.451084	-2.149099	1.373257
1	-2.186873	-1.180531	1.392284
1	-3.327270	1.554480	-1.710154
1	-5.598955	0.546256	-1.762826
8	4.715990	-1.598441	-0.232111
1	5.412220	-2.234368	-0.417531
1	4.029777	-2.063755	0.283285

B			
6	-0.460001	0.695153	0.825750
6	0.535495	1.858601	0.730669
6	1.486459	1.666918	-0.453271
6	2.112375	0.275980	-0.424375
6	0.988326	-0.773571	-0.427315
8	0.156776	-0.570687	0.735458
8	1.247326	1.895957	1.959641
8	2.483582	2.681392	-0.354922
8	2.968232	0.163924	-1.553038
6	1.462318	-2.215006	-0.345922
8	2.282976	-2.465802	0.803614
1	2.009745	2.471762	1.815917
1	3.183178	2.441797	-0.976216
1	1.808213	-2.146583	1.581100
1	-0.947036	0.709666	1.803156
1	-0.036878	2.782866	0.592350
1	0.924247	1.783304	-1.388480
1	2.687511	0.171711	0.500450
1	0.389090	-0.664142	-1.339676
1	3.703484	-0.428231	-1.313513
1	0.590897	-2.877617	-0.333574
1	2.070496	-2.455740	-1.218019
8	-1.405941	0.898891	-0.209883
6	-5.173897	-0.885033	-0.201774
6	-4.853027	0.153927	-1.077349
6	-3.587569	0.728021	-1.055868
6	-2.627137	0.260995	-0.154559
6	-2.930413	-0.786447	0.717071
6	-4.209559	-1.346231	0.688972
1	-6.161812	-1.329770	-0.218105
1	-5.593625	0.523826	-1.777583
1	-3.326061	1.541368	-1.722080
1	-2.182155	-1.180849	1.390200
1	-4.442614	-2.158585	1.368428
8	4.676127	-1.739728	-0.378346
1	5.549857	-1.791008	0.017911
1	4.040634	-2.105201	0.265377

C			
6	0.194663	-0.413584	0.823775
6	-0.892500	-1.490662	0.938668
6	-1.632417	-1.639503	-0.399925
6	-2.125175	-0.278475	-0.892043
6	-0.967544	0.722293	-0.958095
8	-0.316881	0.802695	0.323239
8	-1.799125	-1.217768	1.995517
8	-2.727613	-2.543107	-0.285808
8	-2.705863	-0.364637	-2.190379
6	-1.404650	2.136314	-1.314733
8	-2.434677	2.639597	-0.446489
1	-2.100820	-0.286299	1.987552
1	-3.103132	-2.408484	0.596872
1	-3.290728	2.470301	-0.852622
1	0.593379	-0.172872	1.812163
1	-0.412949	-2.438414	1.190633
1	-0.954942	-2.062336	-1.146621
1	-2.873420	0.091099	-0.180375
1	-0.249501	0.389333	-1.717890
1	-3.288731	-1.134684	-2.184655
1	-1.740677	2.156025	-2.353425
1	-0.550337	2.806347	-1.205770
8	1.212252	-0.953560	-0.003833
6	5.096741	0.560239	-0.059365
6	4.087437	1.317356	0.527314
6	2.770245	0.854793	0.563100
6	2.472710	-0.392944	0.012153
6	3.478475	-1.158913	-0.583014
6	4.782816	-0.680112	-0.618011
1	6.114623	0.930765	-0.085280
1	4.316034	2.286497	0.956751
1	1.991082	1.470598	0.990571
1	3.220486	-2.123574	-1.003293
1	5.558448	-1.281630	-1.078637
8	-2.861587	1.409343	2.085767
1	-2.576522	1.962129	1.333783
1	-2.749154	1.943880	2.877170

(c) Vibrational frequencies.

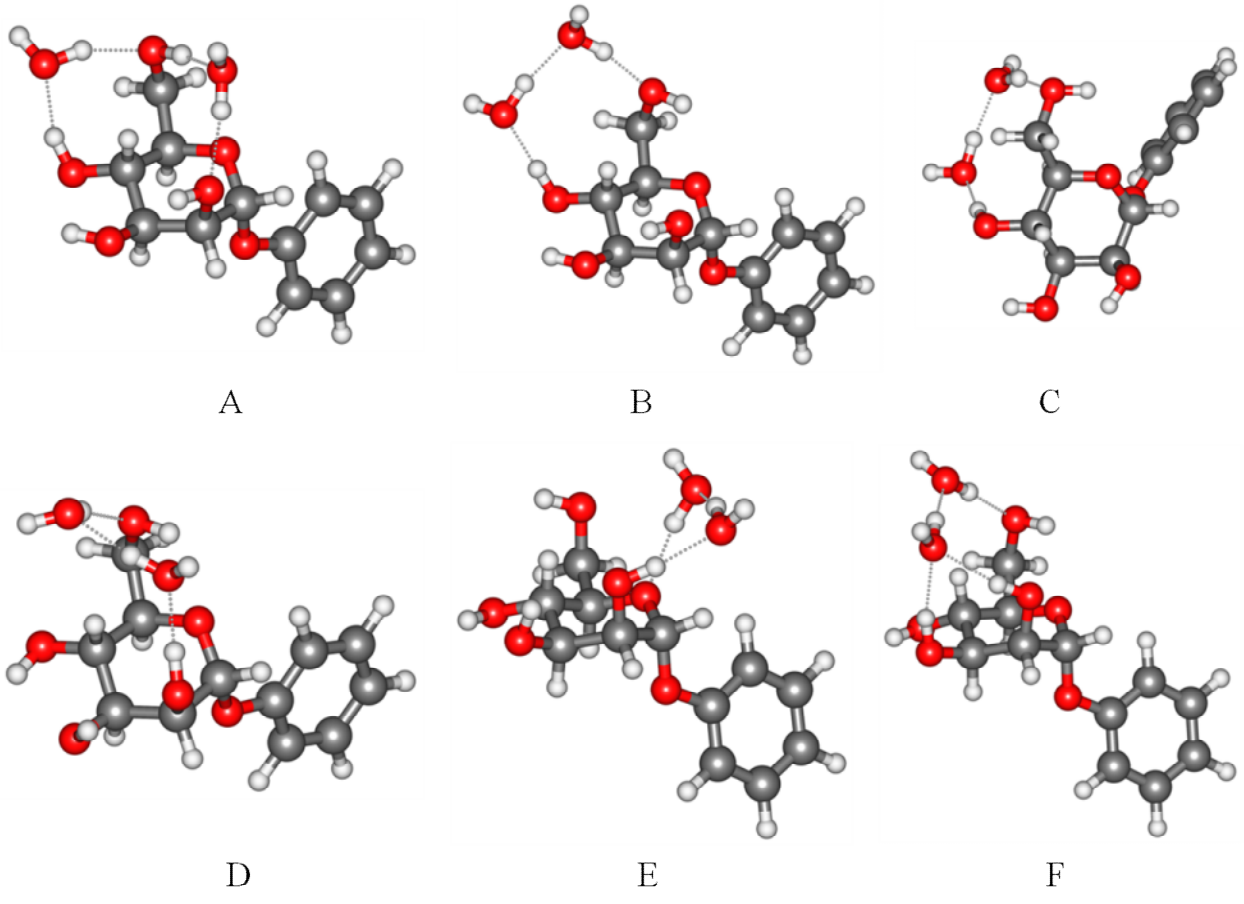
	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
ν1	26.9187	0.2684	27.4912	0.2212	26.1136	0.1066
ν2	41.7231	0.1104	41.8719	0.3699	44.8451	0.1809
ν3	44.6620	0.0857	44.1882	0.0777	45.5112	0.2032
ν4	52.7216	1.6405	53.4486	0.6916	66.4224	3.0513
ν5	95.6712	5.1463	96.2207	4.3115	96.1832	5.4041
ν6	101.7469	2.1609	102.2752	2.0769	107.6955	1.9228
ν7	111.1340	2.6878	112.5937	3.1490	128.4523	2.6369
ν8	139.4608	39.8085	128.8703	75.2494	132.8084	2.3404
ν9	150.2208	26.8475	147.5974	2.7227	150.9763	50.6562
ν10	173.2506	22.6468	170.7173	23.1808	163.0729	10.2213
ν11	206.0262	1.2172	204.1029	3.2323	181.1511	7.8270
ν12	206.8754	7.7373	207.4818	9.5239	208.4931	2.2118
ν13	214.5591	12.9321	212.7545	13.8952	228.0888	15.9646
ν14	251.7929	3.7086	251.4575	4.8615	244.2429	1.4689
ν15	260.6579	10.9743	259.6373	9.5226	255.1495	7.2887
ν16	265.8818	16.7070	264.8588	14.1520	258.3162	32.3979
ν17	274.1038	11.2147	273.7017	11.9070	268.8794	77.1836
ν18	311.8574	39.3198	323.3045	12.5403	279.6959	62.1998
ν19	327.8348	14.6311	343.6109	27.4223	331.0328	12.9300
ν20	366.4431	0.5066	366.3475	0.5161	358.0648	9.3538
ν21	405.0766	19.2265	401.1449	5.3965	376.9738	62.4322
ν22	419.1927	126.8172	421.2726	1.9939	398.0617	30.3942
ν23	421.4585	4.3605	422.9693	29.2988	421.2803	0.0619
ν24	428.7347	74.8869	427.8158	60.4582	426.5540	26.5692
ν25	448.4841	71.7421	444.2563	183.0796	440.2255	5.4182
ν26	455.3956	39.9150	455.6097	38.2889	479.1648	2.8586
ν27	486.6270	19.6626	475.1616	67.1787	495.3174	30.5763
ν28	504.6763	14.2364	486.7245	14.1833	510.9089	3.3531
ν29	519.0614	11.3062	511.7089	42.4331	519.4849	70.3662
ν30	531.4263	39.6758	521.3337	7.1909	522.1798	54.0539
ν31	579.7183	7.9776	579.7031	7.7054	579.6146	1.7444
ν32	618.6165	6.6338	618.6925	7.3891	620.1669	2.8202
ν33	638.4213	10.8034	638.7545	12.9416	640.6036	5.2098
ν34	676.0612	14.6256	677.1972	8.5576	675.5161	3.6694
ν35	685.0226	20.3436	684.8061	24.7320	692.3376	17.8721
ν36	700.3168	24.8693	700.2703	25.2332	701.6619	21.9968
ν37	710.4786	119.5419	726.4555	108.3889	765.1851	55.7300
ν38	764.6409	63.0087	764.6990	62.3770	771.1558	139.1379
ν39	807.8805	19.6209	808.0935	19.2654	810.0929	20.1252
ν40	832.8713	1.7991	832.8090	1.6721	834.6809	1.9170
ν41	842.2771	12.5734	842.7942	9.3016	838.7527	4.4331
ν42	851.0211	21.5876	851.5978	21.3180	847.9239	29.8016
ν43	887.2898	11.9999	887.1803	13.2393	878.4566	46.5140
ν44	903.3527	7.4334	903.3959	7.3385	905.1575	6.1693
ν45	918.0032	12.7937	917.7410	12.4464	913.4031	29.1303
ν46	972.6655	2.2051	972.6661	2.2222	972.4502	56.5922
ν47	985.7875	163.2919	985.7355	168.3669	975.9140	106.8145
ν48	988.7257	25.0869	988.7286	24.0315	988.8245	1.5213
ν49	1010.2267	130.4358	1010.3253	123.0807	1010.9646	83.6128
ν50	1018.4651	235.6605	1018.4821	220.7112	1018.0832	188.0784
ν51	1037.8299	17.6281	1037.7098	22.1140	1029.5600	5.2390
ν52	1044.5648	30.1144	1043.7381	33.8409	1044.0123	11.7534
ν53	1050.5804	119.6775	1050.6480	123.2081	1054.9037	133.0572
ν54	1084.7348	114.4876	1085.6119	113.3831	1078.7438	141.8650
ν55	1100.1750	37.6309	1099.5608	42.9758	1094.0382	76.0350
ν56	1104.4153	67.9679	1103.9375	61.1192	1102.9709	18.4718
ν57	1105.7600	5.1713	1105.6814	9.8316	1109.0007	102.6222
ν58	1120.6007	84.3732	1120.3405	81.8621	1116.7486	35.3047
ν59	1129.4665	46.9193	1129.7598	45.9689	1127.7679	65.6997
ν60	1134.8613	8.9400	1133.7715	7.2625	1150.0239	9.6317
ν61	1178.8323	3.6127	1178.8675	3.6000	1178.8967	4.4071
ν62	1184.6265	35.0965	1188.5817	29.4157	1196.0349	30.0021
ν63	1195.1422	19.4807	1195.1118	20.1448	1197.4617	14.5503
ν64	1223.3120	58.6182	1223.8301	69.0437	1226.0558	85.6478
ν65	1229.3882	35.2233	1229.9921	38.2952	1244.1825	271.5123
ν66	1247.1525	241.9549	1246.9831	238.8197	1245.8788	36.5804
ν67	1258.0815	59.4281	1258.0836	59.3159	1268.0101	31.3440
ν68	1270.1904	13.8199	1269.0831	13.5333	1294.3156	44.8753
ν69	1304.6249	6.9149	1301.0354	8.3126	1309.7326	10.8787
ν70	1324.3630	3.7914	1323.8397	3.5135	1322.5553	6.7475
ν71	1341.3390	3.8840	1340.9999	3.2954	1332.1485	16.5831
ν72	1348.6333	22.5852	1347.0790	20.8100	1348.9609	5.5202
ν73	1354.6757	5.3889	1354.6156	6.6277	1355.1308	4.1990

v74	1362.1322	5.7411	1362.3274	7.7050	1356.3950	1.1604
v75	1375.2218	30.7554	1374.6605	30.7872	1370.2828	35.5374
v76	1392.7113	12.1735	1392.7811	12.0328	1385.4361	7.5930
v77	1406.1947	3.4507	1404.8349	8.8611	1397.9807	12.0243
v78	1415.3766	32.6429	1415.6659	36.1905	1410.1889	4.2576
v79	1417.7433	44.4427	1416.9958	36.7656	1424.4568	39.5161
v80	1427.5127	20.5854	1428.2483	21.0410	1428.0216	4.1847
v81	1436.1156	9.5969	1436.4857	7.6684	1445.8443	36.9182
v82	1463.6622	24.1582	1457.7326	22.6079	1447.2290	28.0561
v83	1486.4342	1.2568	1486.4360	1.2414	1485.1088	9.5689
v84	1495.8693	7.9751	1499.2127	8.1233	1486.5382	0.7128
v85	1522.1052	112.4231	1522.1212	112.2746	1522.2630	109.7207
v86	1626.2306	26.4321	1626.3026	26.5720	1626.5554	25.2892
v87	1639.8006	67.3449	1639.8030	66.9489	1639.6901	65.9063
v88	2604.3968	182.5936	2613.5514	163.4018	2612.9104	171.5001
v89	2842.2674	86.0253	2845.7936	89.3311	2836.1344	74.1240
v90	3014.2124	10.3190	3015.3442	9.8242	3016.6790	2.2048
v91	3021.9078	6.0169	3023.2426	4.7944	3029.2753	23.8303
v92	3030.4205	41.4858	3031.2675	39.6149	3064.8725	25.1910
v93	3041.7942	40.5788	3041.5776	38.3494	3069.6415	10.4065
v94	3060.5691	22.7314	3056.8594	29.2784	3074.1780	26.3697
v95	3082.1783	16.9749	3081.3377	17.1650	3086.3629	29.3062
v96	3117.7642	11.4459	3118.6151	9.0423	3115.2737	12.7294
v97	3165.4623	1.2724	3165.5266	1.2459	3165.7195	1.1604
v98	3173.1530	11.3513	3173.2419	11.3146	3173.5616	11.2029
v99	3188.1574	19.7166	3188.1987	19.7405	3188.1717	19.3390
v100	3195.3417	7.3682	3195.4034	7.2939	3195.5977	7.3392
v101	3213.6950	1.3478	3213.6157	1.3190	3213.6306	0.9403
v102	3625.9082	510.4203	3627.1851	517.3581	3532.0722	501.8777
v103	3784.5750	88.4870	3786.4741	88.4935	3742.6186	61.4428
v104	3792.0949	51.9035	3792.5997	49.5342	3791.8093	64.4906
v105	3802.8238	51.2976	3803.8380	50.7602	3840.9223	58.0393

3. α-PhMan•$(D_2O)_2$

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

Conformer	B3LYP/6-311++G(d,p) energy / kJ mol^{-1}	MP2/6-311++G(d,p)//B3LYP/6-311++G(d,p) energy / kJ mol^{-1}
A	0.00	0.00
B	0.86	9.77
C	10.34	13.83
D	10.00	14.15
E	13.07	14.63
F	10.88	14.88



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

A			
6	-0.596132	0.548233	0.819227
6	0.381900	1.721489	0.909813
6	1.215632	1.820222	-0.365704
6	1.877879	0.483156	-0.687084
6	0.820889	-0.635520	-0.744541
8	0.048317	-0.650027	0.477381
8	1.221183	1.479965	2.046855
8	2.197115	2.831050	-0.138520
8	2.570746	0.634217	-1.918407
6	1.408793	-2.036570	-0.879517
8	2.488773	-2.309377	0.012571
1	1.959203	2.101016	1.969858
1	2.840061	2.760242	-0.856064
1	2.256289	-2.064563	0.931524
1	-1.052201	0.362822	1.795154
1	-0.184137	2.645556	1.060938
1	0.561620	2.107306	-1.197480
1	2.587294	0.253101	0.112495
1	0.153976	-0.459318	-1.597340
1	3.374986	0.082469	-1.878510
1	0.601582	-2.762874	-0.735873
1	1.804715	-2.160490	-1.889143
8	-1.582629	0.935054	-0.122305
6	-5.328934	-0.884168	-0.303771
6	-4.309875	-1.511392	0.406443
6	-3.036182	-0.944595	0.488447
6	-2.795653	0.277072	-0.142611
6	-3.810312	0.912575	-0.862591
6	-5.069756	0.330077	-0.942078
1	-6.312079	-1.335661	-0.364320
1	-4.495320	-2.459737	0.898433
1	-2.244678	-1.462276	1.012824
1	-3.595031	1.858725	-1.344486
1	-5.853387	0.829886	-1.500413
8	4.616675	-1.127969	-1.211192
1	4.013695	-1.698875	-0.686467
1	5.225502	-1.709883	-1.674045
8	2.097303	-1.266533	2.603427
1	2.787461	-1.223550	3.271774
1	1.761098	-0.358417	2.496467

B			
6	-0.862965	0.614875	0.910769
6	0.030619	1.856841	0.984147
6	0.945121	1.928032	-0.237901
6	1.706791	0.618913	-0.440653
6	0.707351	-0.547606	-0.523304
8	-0.138424	-0.566217	0.648184
8	0.781001	1.760876	2.187214
8	1.843358	3.014233	-0.022925
8	2.454950	0.738265	-1.641173
6	1.353910	-1.924305	-0.547604
8	2.033029	-2.209445	0.682765
1	1.488960	2.414819	2.120174
1	2.522983	2.952665	-0.706370
1	1.447547	-1.936344	1.401703
1	-1.345380	0.447588	1.876371
1	-0.617992	2.740127	1.007051
1	0.334102	2.116260	-1.129543
1	2.371184	0.460406	0.414744
1	0.096638	-0.430674	-1.426295
1	3.358458	0.388378	-1.502268
1	2.094680	-1.976968	-1.345726
1	0.586495	-2.684351	-0.727374
8	-1.827300	0.880856	-0.092329
6	-5.438328	-1.185716	-0.352091
6	-4.431167	-1.691548	0.463876
6	-3.201251	-1.039569	0.575626
6	-2.992532	0.144873	-0.133052
6	-3.996130	0.658114	-0.958941
6	-5.211064	-0.007946	-1.066549
1	-6.387196	-1.702254	-0.435026
1	-4.591108	-2.610265	1.017295
1	-2.416346	-1.465274	1.185038
1	-3.807505	1.577979	-1.499319
1	-5.985872	0.398172	-1.707142
8	5.006818	-0.201526	-1.146655
1	5.053126	-0.952974	-0.516317
1	5.592817	-0.422597	-1.876111
8	4.785307	-2.306421	0.586693
1	5.212581	-2.404004	1.442242
1	3.819782	-2.345412	0.746725

C			
6	0.062916	-1.561708	0.456839
6	-1.156536	-2.259562	-0.158860
6	-2.124050	-1.236526	-0.760978
6	-2.446550	-0.120196	0.236190
6	-1.133085	0.516961	0.702906
8	-0.279704	-0.483722	1.295800
8	-1.775581	-3.003360	0.879210
8	-3.304318	-1.946290	-1.131117
8	-3.347048	0.818506	-0.334459
6	-1.314855	1.587585	1.762616
8	-0.093318	2.308449	1.991912
1	-2.653851	-3.244257	0.556418
1	-3.995155	-1.286943	-1.277032
1	0.584809	1.664675	2.230955
1	0.597909	-2.267871	1.095011
1	-0.797786	-2.929732	-0.949092
1	-1.659659	-0.790419	-1.650265
1	-2.961060	-0.555778	1.097341
1	-0.618981	0.956927	-0.159927
1	-2.865226	1.411025	-0.947221
1	-1.664643	1.132719	2.695157
1	-2.049525	2.320454	1.432220
8	0.875036	-1.149117	-0.632800
6	4.866287	-0.028922	-0.190323
6	4.251224	-0.090622	-1.442373
6	2.917046	-0.462298	-1.555467
6	2.181245	-0.778219	-0.409278
6	2.782496	-0.710681	0.849791
6	4.126216	-0.341228	0.945660
1	5.907387	0.258549	-0.104290
1	4.814781	0.147535	-2.337628
1	2.428184	-0.522201	-2.520441
1	2.221786	-0.931613	1.747548
1	4.590105	-0.296126	1.924847
8	0.085625	3.836919	-0.342025
1	0.165602	3.391736	0.526362
1	0.983247	3.998016	-0.647165
8	-1.860655	2.625839	-1.911784
1	-1.168411	3.116064	-1.419208
1	-2.333925	3.281943	-2.431812

D			
6	-0.521356	0.429843	0.800061
6	0.452671	1.604102	0.973753
6	1.142789	1.925587	-0.360458
6	1.750754	0.664733	-0.978086
6	0.682316	-0.422560	-1.118437
8	0.085284	-0.679087	0.170072
8	1.405174	1.366790	1.998213
8	2.145427	2.923654	-0.191849
8	2.284260	0.930267	-2.271098
6	1.221557	-1.767178	-1.586079
8	2.148315	-2.331165	-0.654727
1	1.834264	0.491011	1.921126
1	2.538297	2.771737	0.680232
1	1.757843	-2.268926	0.229412
1	-0.847552	0.063333	1.776275
1	-0.120942	2.474227	1.298464
1	0.408143	2.335905	-1.058930
1	2.545908	0.293892	-0.319568
1	-0.083551	-0.086068	-1.826850
1	2.775599	1.758922	-2.205256
1	0.383352	-2.455706	-1.738372
1	1.751794	-1.640209	-2.529814
8	-1.622435	0.928012	0.060800
6	-5.339710	-0.959277	0.018307
6	-5.172366	0.346376	-0.446780
6	-3.920130	0.948645	-0.419501
6	-2.820081	0.242339	0.073552
6	-2.970301	-1.068712	0.528572
6	-4.237009	-1.656068	0.502702
1	-6.317112	-1.426534	-0.001091
1	-6.022144	0.901728	-0.827561
1	-3.775045	1.964275	-0.767630
1	-2.117106	-1.636116	0.873590
1	-4.351618	-2.674182	0.857877
8	4.687967	-1.721914	0.212065
1	3.931465	-1.983287	-0.350721
1	5.288207	-1.215805	-0.342794
8	2.869475	-1.035214	2.145881
1	3.110203	-1.250135	3.051993
1	3.667460	-1.195802	1.599128

E			
6	-0.129167	0.059835	-0.738133
6	0.965837	-0.590994	-1.603932
6	1.716112	-1.653231	-0.795085
6	2.207567	-1.051224	0.524984
6	1.035175	-0.467649	1.315350
8	0.365318	0.524142	0.506787
8	1.950133	0.338534	-2.023582
8	2.817797	-2.183655	-1.527637
8	2.840727	-2.033543	1.339433
6	1.436005	0.206453	2.621815
8	2.387260	1.259622	2.454014
1	1.556069	1.184607	-2.314700
1	3.221042	-1.438066	-1.994684
1	3.264115	0.870514	2.377019
1	-0.532976	0.945373	-1.234160
1	0.473613	-1.056657	-2.466282
1	1.054086	-2.495693	-0.581748
1	2.910005	-0.243655	0.285491
1	0.328579	-1.270983	1.556165
1	3.412830	-2.550232	0.757508
1	0.549732	0.665061	3.064403
1	1.811893	-0.558433	3.306835
8	-1.133042	-0.921530	-0.572246
6	-5.056031	0.012835	0.487538
6	-4.075003	0.991893	0.610527
6	-2.745839	0.723989	0.276083
6	-2.408572	-0.543162	-0.201179
6	-3.384895	-1.534722	-0.324197
6	-4.701595	-1.254436	0.021452
1	-6.083324	0.230604	0.754538
1	-4.334644	1.978048	0.978960
1	-1.993285	1.488770	0.409272
1	-3.095041	-2.510030	-0.696419
1	-5.454643	-2.027994	-0.079210
8	1.072598	3.268557	0.355419
1	0.914610	2.332426	0.578559
1	1.811192	3.521060	0.918700
8	0.839457	2.842982	-2.332375
1	0.994772	3.207289	-1.433325
1	0.911832	3.569584	-2.956763

F			
6	-0.572041	-0.380275	-0.800514
6	0.559398	-1.417667	-0.795578
6	1.171107	-1.471683	0.611671
6	1.624106	-0.085006	1.059947
6	0.531224	0.977814	0.886749
8	-0.119510	0.893149	-0.394334
8	1.448673	-0.996448	-1.818017
8	2.239421	-2.406528	0.744659
8	1.982852	-0.076549	2.440893
6	1.107239	2.389589	0.926482
8	1.964464	2.630527	-0.200537
1	2.352531	-1.310929	-1.660862
1	2.994290	-2.114154	0.205822
1	1.458275	2.377590	-0.985589
1	-0.940652	-0.238220	-1.818603
1	0.133145	-2.399288	-1.034551
1	0.391952	-1.826764	1.290676
1	2.490088	0.203631	0.457768
1	-0.203527	0.857907	1.691020
1	2.504435	-0.873015	2.600686
1	0.294611	3.123004	0.931138
1	1.710986	2.519761	1.824281
8	-1.596701	-0.880635	0.038258
6	-5.534164	0.474017	-0.161295
6	-5.189973	-0.687841	0.532156
6	-3.868252	-1.114656	0.579478
6	-2.874886	-0.374827	-0.067564
6	-3.203291	0.796304	-0.752778
6	-4.537385	1.206349	-0.798705
1	-6.565561	0.803944	-0.199543
1	-5.955304	-1.268722	1.034658
1	-3.585894	-2.018419	1.106010
1	-2.436223	1.396066	-1.222680
1	-4.789695	2.115564	-1.333144
8	4.474991	1.455804	-0.644715
1	3.637623	1.931041	-0.458277
1	5.163466	1.916051	-0.156371
8	4.198238	-1.258788	-1.054345
1	4.402385	-0.303468	-0.938889
1	4.925147	-1.648544	-1.548734

(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	26.5312	0.1109	20.5769	0.3374	17.1581	1.0625
v2	42.9959	0.3496	26.9922	0.5314	30.5872	0.9600
v3	45.1067	0.2532	32.4881	0.2290	35.7666	1.3871
v4	55.1400	1.5947	37.3977	0.8241	42.1145	0.6771
v5	57.5281	1.3706	46.1202	0.1628	53.0951	0.7280
v6	104.4576	1.3910	72.7271	2.4415	72.3231	4.6738
v7	113.2859	2.0022	95.8980	1.1268	92.6562	2.7051
v8	117.9024	0.6728	100.9356	3.1605	109.4136	6.5599
v9	131.5462	1.2449	109.1842	3.6508	113.8000	3.1949
v10	157.9734	3.5163	147.9100	5.3544	139.7383	8.9758
v11	166.9303	9.2904	154.0232	53.5015	150.3676	55.7303
v12	172.9765	14.7304	173.4882	15.2255	166.2476	10.2218
v13	177.8000	56.1604	183.9491	40.7538	182.8324	23.9334
v14	192.0729	70.2400	204.2455	25.3073	198.3808	10.6410
v15	214.5220	1.2333	211.0328	10.2703	202.6260	30.3399
v16	222.4909	32.1128	224.8238	13.1739	215.2114	10.4725
v17	246.8007	19.9748	246.9918	10.0178	240.7301	6.4847
v18	257.2031	13.1127	254.1496	19.7059	242.5498	4.8927
v19	264.3224	11.0344	257.7420	5.0520	256.8582	12.1452
v20	270.4909	40.9552	264.7079	10.7383	270.0879	21.8089
v21	285.1303	4.0427	273.7327	21.5072	306.6092	5.1208
v22	309.4055	4.2069	328.9513	3.4048	312.8527	3.9885
v23	336.1723	28.1547	340.8230	9.7011	335.9616	9.9236
v24	352.4605	17.7154	347.0986	46.8122	348.9566	17.3370
v25	369.4340	1.8229	366.4048	0.4931	363.9571	2.6425
v26	414.3594	11.1604	416.5658	34.0547	395.2859	1.8463
v27	421.3106	0.1948	421.5942	2.5160	416.5754	25.3786
v28	427.9797	19.1023	422.6814	43.5293	421.4344	0.0422
v29	440.4260	29.9826	437.8841	189.7819	440.1113	49.9287
v30	458.2203	63.4253	448.3653	39.8248	454.7092	55.8220
v31	478.6476	20.8445	452.6960	19.8760	460.0025	84.2759
v32	505.1529	3.2973	482.2203	27.1347	466.7175	51.0330
v33	516.8509	120.8667	490.6201	41.7060	518.0896	93.5289
v34	523.5196	58.2370	511.6528	51.8960	519.8947	46.9547
v35	559.8491	34.8639	521.9360	5.9795	532.9399	35.5822
v36	583.1172	9.4463	580.9475	9.0549	564.2293	41.6951
v37	618.8787	3.0113	608.2659	56.7180	576.7345	42.0419
v38	639.0433	7.3988	618.1102	6.7525	604.5825	12.0616
v39	675.0913	10.9483	636.9385	7.5014	625.6231	0.4116
v40	688.5734	34.5672	676.5227	15.1512	664.4613	46.2805
v41	701.8532	25.2939	681.5146	22.1891	691.1709	14.0781
v42	730.8395	49.0226	701.8512	24.3478	702.1286	22.5283
v43	765.5094	64.0339	759.2818	114.6089	752.4489	124.6803
v44	768.4914	164.3696	765.6345	57.2840	766.5722	71.0894
v45	809.8792	18.1281	810.8186	16.1520	800.6269	17.6890
v46	833.8205	5.8866	835.9634	1.2814	825.9088	16.5444
v47	836.9165	4.5739	848.7442	13.8019	836.1706	2.8278
v48	854.6028	17.3064	857.7544	17.6574	846.7736	17.3726
v49	889.4758	14.4161	889.6210	13.9995	889.0286	11.9542
v50	906.8927	7.1784	905.7861	7.3881	903.6475	5.4719
v51	921.8194	8.6741	917.7494	15.5101	972.3682	71.5422
v52	974.2673	1.4156	974.3535	2.3694	976.1430	30.5896
v53	988.6176	73.3447	988.3478	131.8615	991.5350	0.7740
v54	990.8027	72.4981	990.4197	71.1214	1008.7520	92.8274
v55	1011.4159	60.4395	1011.0007	91.6526	1012.0220	57.6126
v56	1025.7724	307.1945	1019.2534	216.9936	1019.0417	242.7899
v57	1045.1555	24.4270	1037.1181	44.0088	1045.9499	19.8619
v58	1049.6878	56.5703	1045.9707	44.4958	1047.2892	44.8279
v59	1054.1344	120.7154	1050.8285	124.4672	1057.5912	82.5458
v60	1085.6771	115.8760	1087.1908	132.4155	1077.2923	118.6852
v61	1090.7088	51.6319	1101.7733	30.8298	1102.0164	58.8293
v62	1103.8370	25.5699	1104.5934	42.9065	1106.9297	73.8615
v63	1108.1067	2.1302	1105.9408	22.5942	1113.2328	10.8530
v64	1124.6041	105.1671	1118.4612	55.4348	1125.0623	87.5194
v65	1130.4708	57.0695	1125.4044	63.1267	1129.5583	18.4954
v66	1137.9887	2.8182	1130.1813	18.9004	1144.6167	26.6711
v67	1178.8561	3.7242	1179.0098	3.5948	1179.0599	3.6299
v68	1189.2550	34.7503	1195.9385	17.1316	1197.1296	18.1061
v69	1196.2753	34.1881	1200.1898	27.6740	1206.9028	22.6891
v70	1199.2666	21.9355	1215.0552	8.9894	1213.3873	11.2511
v71	1230.7846	52.7064	1227.5585	74.8651	1227.7557	13.1564
v72	1246.0479	226.5712	1236.5852	43.0937	1235.0137	75.7375
v73	1255.5085	48.7548	1248.4024	222.9023	1249.4375	213.7765

v74	1263.4645	18.1408	1257.9579	60.8906	1258.5672	63.6968
v75	1276.6963	32.0582	1267.3133	16.6283	1270.9138	11.8545
v76	1310.3067	5.2950	1305.4096	9.0818	1302.3361	15.3802
v77	1326.3002	4.9995	1324.0703	4.7302	1327.0360	7.4091
v78	1341.1782	1.3181	1337.5165	1.8264	1343.7203	5.0001
v79	1349.5483	23.0079	1345.8204	21.5550	1348.4666	15.0114
v80	1355.7465	4.3708	1354.9028	11.0612	1356.0134	8.1159
v81	1371.4295	13.6448	1359.5030	7.6241	1373.4610	24.0272
v82	1381.6235	18.3434	1374.5224	29.7282	1387.3105	7.0019
v83	1395.8503	9.8895	1395.9733	13.8247	1396.2368	23.2726
v84	1407.3913	5.3123	1408.1892	4.2089	1400.7666	5.8559
v85	1413.5435	15.6731	1414.6267	22.1297	1414.4028	15.1562
v86	1421.7671	54.5804	1418.9615	54.2118	1426.5880	35.4690
v87	1435.1378	22.2201	1431.4222	41.9146	1434.8474	23.7008
v88	1455.6542	47.3552	1437.1633	2.8740	1438.7885	11.2658
v89	1475.5226	27.8233	1480.0731	20.7496	1474.1520	53.9960
v90	1486.7980	1.8145	1486.5495	1.3740	1486.4469	1.1372
v91	1497.8886	7.0479	1502.7462	8.8924	1501.9680	5.6328
v92	1522.6457	110.6616	1522.3837	113.0052	1523.3702	107.9571
v93	1626.7585	26.5131	1626.4612	26.3738	1625.9061	27.3811
v94	1639.9260	66.2513	1639.9959	68.6012	1640.0123	67.4672
v95	2522.3166	285.9307	2519.8104	297.0457	2536.1034	278.0329
v96	2634.9940	165.1091	2574.0829	402.6263	2578.2128	242.4167
v97	2836.8663	55.4104	2832.1336	62.4526	2829.9505	60.0712
v98	2837.0163	100.6388	2835.8959	84.3928	2832.4277	62.0854
v99	3023.2833	4.7470	3017.4484	9.3896	3009.2611	12.3834
v100	3029.9820	7.3598	3027.5984	6.5541	3024.2914	40.7393
v101	3035.6933	50.3404	3030.0555	39.5841	3029.5056	2.4029
v102	3053.0148	27.9128	3040.0398	31.6145	3043.5757	21.9289
v103	3064.2512	26.9696	3053.2681	37.9102	3067.4766	37.2545
v104	3071.3456	20.4505	3080.7741	18.0276	3085.3029	18.7416
v105	3099.2022	20.6550	3117.0975	11.4641	3133.7344	7.3791
v106	3165.5454	1.0024	3165.7687	1.1955	3165.3037	1.4996
v107	3173.4570	11.1546	3173.6134	11.2303	3172.7408	10.9752
v108	3187.8034	19.7607	3188.2364	19.9351	3188.4333	18.5706
v109	3195.1680	7.1858	3195.6760	7.3218	3195.5077	6.6143
v110	3210.2632	0.4789	3215.6546	1.4236	3210.7823	2.3912
v111	3542.7160	459.0644	3518.7304	971.8625	3531.7196	511.9989
v112	3581.8086	600.7058	3782.3529	65.4807	3784.8820	108.4055
v113	3767.3012	88.9784	3787.5284	91.3191	3788.1305	33.3257
v114	3791.2384	62.6687	3793.3167	49.3007	3806.1911	56.0754

	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	24.1337	0.1743	27.8324	0.4317	25.7919	0.6774
v2	31.9759	0.6542	36.4995	1.4565	40.3901	0.8525
v3	39.4021	1.2432	41.2659	1.7827	43.6256	0.3541
v4	44.2405	0.1623	48.7591	0.6507	48.2946	2.3086
v5	47.0628	0.2580	57.0586	2.3384	76.0493	2.1588
v6	70.1147	0.4946	67.6793	2.3207	80.5231	0.0451
v7	99.5209	2.8703	93.0005	5.8273	94.2947	3.1569
v8	110.4005	5.8818	99.4846	7.5554	107.7158	2.0339
v9	118.1747	10.2130	115.5550	1.4530	119.7656	13.4829
v10	134.6753	0.2299	130.7334	53.9164	130.0731	49.9013
v11	165.4915	10.5604	140.9946	12.0512	148.7800	5.4496
v12	176.7405	69.6894	142.0983	6.4580	165.5212	26.7982
v13	187.6450	15.7754	166.4348	9.0281	178.6987	29.1346
v14	201.8398	2.2540	198.3937	18.3402	190.0454	8.0136
v15	211.7669	8.4643	204.2008	1.5927	206.7993	3.0349
v16	218.3249	4.3503	211.0375	8.9463	219.9405	8.9000
v17	246.7093	8.4976	222.5097	22.5329	244.2880	9.2370
v18	252.2087	10.0214	250.2634	5.4416	248.4684	12.6193
v19	256.3697	21.9440	257.7935	7.6495	258.9067	21.3237
v20	261.4018	12.1546	263.3452	23.5531	269.6191	3.3496
v21	272.4123	15.7358	271.3290	8.4457	290.4063	7.5316
v22	313.4867	42.9985	299.8819	10.7755	314.8470	8.5195
v23	328.3313	34.5464	327.6897	114.5135	332.1191	5.7856
v24	334.5646	17.1287	338.7812	4.3297	363.8115	20.1816
v25	359.4065	5.9911	358.9956	40.4086	373.3155	53.0005
v26	392.9037	11.1439	367.0645	23.5217	381.8008	50.5933
v27	415.7239	47.1528	400.5823	8.4737	420.8081	0.1274
v28	421.4691	0.0751	421.2753	0.2725	424.8111	23.8519
v29	439.3807	6.3141	423.9316	47.0136	443.4822	5.2017
v30	458.7930	54.7509	443.3168	2.8522	474.4817	35.7226
v31	480.4013	3.7060	484.6740	4.2381	484.1099	62.3563
v32	505.5967	12.9432	497.9621	61.2170	509.1877	59.1571
v33	513.8063	132.8893	511.3720	16.3877	519.0780	29.8757
v34	520.5825	10.2090	519.6302	21.0386	524.8439	72.3744
v35	538.4175	203.9625	531.1563	114.7866	546.3749	59.6060
v36	578.6254	5.2987	534.3747	125.4979	583.6220	10.6448
v37	603.8653	26.0860	580.6166	1.1852	619.0607	20.2893
v38	621.7488	10.9421	619.4570	4.1745	624.8774	7.0671
v39	641.6128	14.0620	639.8048	4.1014	640.0447	13.3440
v40	676.2888	3.3356	672.7102	19.2823	674.8767	8.5618
v41	688.5861	17.0833	690.8711	11.0844	686.6180	9.2493
v42	701.8690	22.2606	700.3572	22.3749	701.9778	12.2624
v43	766.2752	63.2574	735.7525	90.8505	704.5584	181.7440
v44	779.4575	123.6425	764.4500	68.0122	765.6292	66.9505
v45	809.6887	16.9123	808.8589	16.8854	807.0677	18.2445
v46	836.3464	1.0701	832.8907	2.0685	835.0785	1.1349
v47	845.1778	15.9236	839.3722	5.3472	850.0337	33.9329
v48	860.1749	34.1953	850.2356	26.7901	865.7284	25.4831
v49	876.6358	44.5380	889.8894	59.8329	891.8539	12.9807
v50	906.0508	4.8836	903.4554	11.2926	905.0141	5.4085
v51	913.6889	18.6404	914.0690	33.8890	909.8037	17.7978
v52	974.9204	4.3822	972.5576	98.4647	973.1820	0.7258
v53	983.0520	129.8278	975.2526	51.3744	987.5402	25.0348
v54	990.4947	3.5123	990.1473	0.8349	989.5411	20.5672
v55	1011.4758	82.3478	1012.3573	16.9580	1011.1824	161.4244
v56	1018.0243	222.7691	1024.7731	233.9018	1014.4561	125.9317
v57	1036.3460	10.9905	1033.5078	2.7031	1034.5097	127.7143
v58	1043.5910	2.5641	1044.3836	12.4035	1044.8076	7.0636
v59	1055.5538	120.3294	1060.8086	190.0340	1052.3973	192.3306
v60	1088.3738	143.7426	1079.4831	109.2509	1076.9101	158.1908
v61	1095.8837	79.2070	1092.3295	36.3856	1099.3427	28.0896
v62	1102.2503	45.3667	1101.3926	56.8331	1103.1568	39.1044
v63	1105.3773	64.4713	1105.0335	111.7145	1105.3475	8.7593
v64	1115.1616	27.2236	1111.2070	50.1859	1110.7802	18.9126
v65	1127.4416	81.5551	1126.1980	14.8116	1123.0541	122.6239
v66	1156.5116	31.5274	1144.4679	16.4956	1162.5037	69.5124
v67	1179.0941	4.1510	1178.7409	4.5063	1178.7789	3.4902
v68	1192.1406	44.5920	1195.3735	20.9793	1197.4302	13.3133
v69	1196.3103	21.3409	1200.5055	61.3920	1208.3696	33.1104
v70	1211.4316	22.9682	1217.0561	22.1532	1216.1282	41.0749
v71	1230.4673	41.5076	1222.5706	73.5018	1233.5421	32.8083
v72	1243.2983	342.8678	1242.0489	247.7269	1243.3334	56.7166
v73	1249.0648	6.9488	1249.3312	56.5293	1249.7711	225.3892

v74	1265.3035	23.3843	1257.6959	22.1747	1273.5416	57.1901
v75	1290.3773	54.8056	1283.2419	58.4747	1295.5765	7.2195
v76	1308.9851	17.9068	1315.6671	21.6861	1314.4367	10.6464
v77	1321.0720	10.0816	1325.4323	10.1486	1326.6300	0.8334
v78	1330.5418	7.9625	1340.4810	10.8704	1331.0481	14.1589
v79	1341.2735	1.1315	1347.6274	15.1258	1343.0764	11.4668
v80	1346.7972	5.3400	1354.1300	6.4969	1355.3147	6.0459
v81	1355.5494	2.4102	1356.0061	0.5857	1359.8385	37.7020
v82	1366.7751	28.8040	1379.6439	13.8940	1371.1743	15.8915
v83	1377.6296	17.2411	1390.7869	9.9519	1379.8217	11.4051
v84	1398.4923	22.8173	1402.2470	24.2092	1401.6779	8.2488
v85	1419.4414	2.5036	1411.8565	26.4590	1410.6116	45.3805
v86	1422.1338	28.6582	1419.0137	10.8738	1421.3881	4.5657
v87	1431.8545	18.1939	1430.1844	48.6166	1427.4132	23.8197
v88	1436.3653	92.3757	1446.0555	3.8582	1446.8532	10.3555
v89	1444.4629	11.9536	1456.7405	11.6350	1471.7292	38.5605
v90	1486.3533	0.6616	1486.4809	0.5605	1486.3981	1.3879
v91	1497.9536	8.7761	1486.9461	10.2073	1502.1100	7.8489
v92	1522.6590	108.5811	1521.7084	105.0316	1522.6821	113.5181
v93	1626.8740	24.9325	1626.8880	25.8459	1626.5525	25.8937
v94	1639.8795	66.5581	1639.6675	60.8949	1639.9633	70.6699
v95	2540.5773	193.2439	2523.0867	259.2785	2505.3883	352.0340
v96	2589.2631	347.7911	2632.5898	245.9405	2556.4570	304.9333
v97	2829.2600	65.8483	2826.2268	75.0514	2831.9456	62.9335
v98	2836.4574	68.6989	2840.2627	69.0092	2833.6404	85.7902
v99	3017.8748	10.7767	3017.0655	10.1379	3021.5180	38.6634
v100	3028.7278	16.6160	3019.7463	31.6313	3032.6399	7.5023
v101	3041.3153	44.8733	3033.4075	14.5257	3044.4663	41.6670
v102	3067.1672	15.7627	3054.0364	35.0381	3062.3081	9.3691
v103	3075.1388	21.4667	3080.0296	4.9053	3080.9880	13.6572
v104	3086.4402	28.1273	3081.9509	23.1929	3082.2071	33.9168
v105	3121.2861	8.5504	3104.3404	14.2758	3124.8217	8.8994
v106	3166.2299	1.1433	3165.9658	0.9958	3165.0412	1.2414
v107	3174.0558	10.7968	3174.2488	10.4380	3172.9518	11.4999
v108	3188.4872	19.0607	3187.9509	19.7171	3187.6393	20.5152
v109	3195.9064	7.4828	3195.2188	7.3188	3195.2058	7.3397
v110	3213.1942	1.1361	3210.1024	0.6623	3212.7321	1.2890
v111	3551.3700	516.9277	3547.0112	657.9522	3651.4635	100.3094
v112	3743.5269	54.5113	3760.6284	61.1476	3700.8432	598.3603
v113	3752.4831	78.1493	3788.8615	63.6516	3765.9485	63.6841
v114	3793.6852	61.0403	3838.3566	40.6930	3796.3517	57.5118

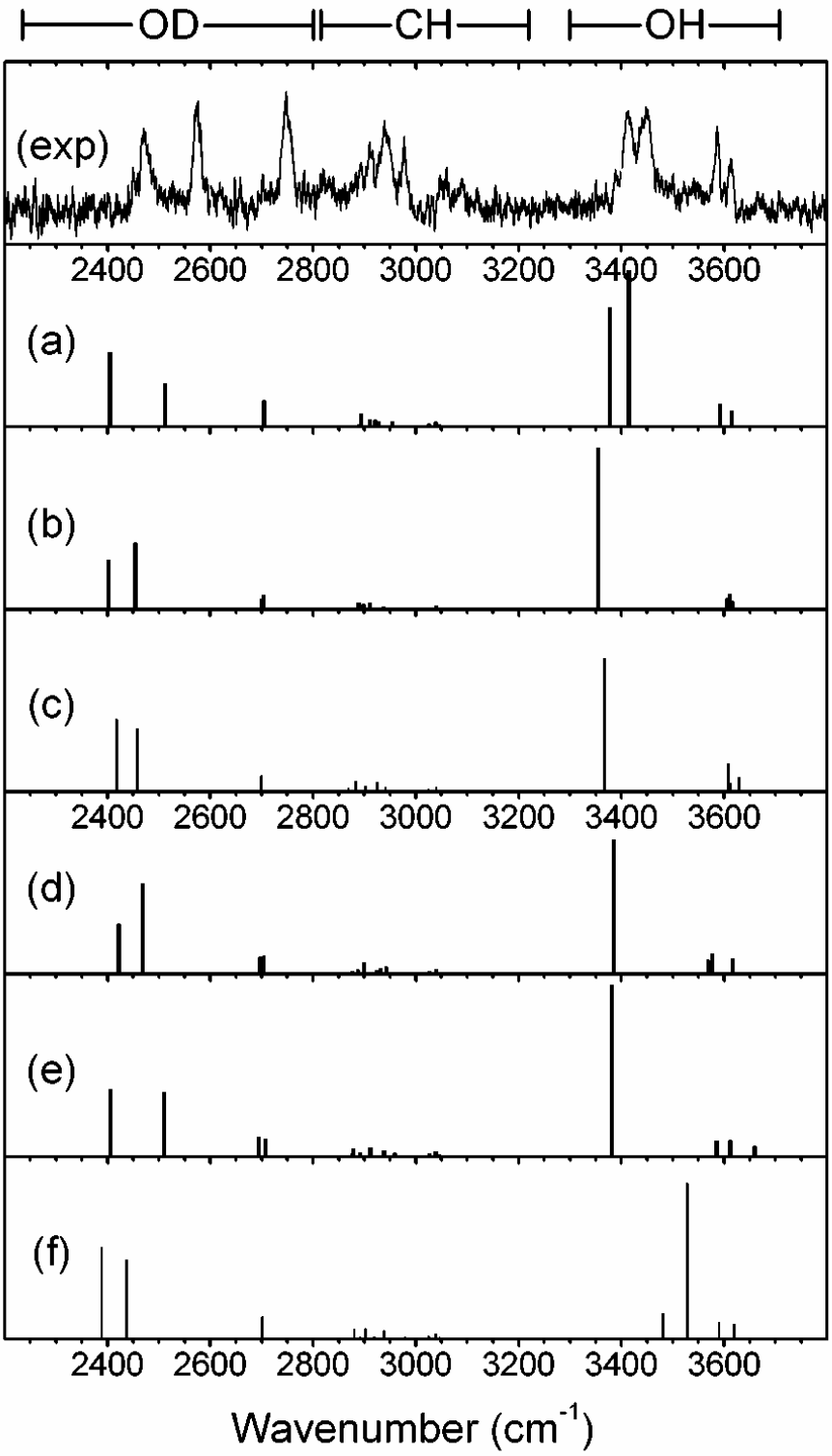
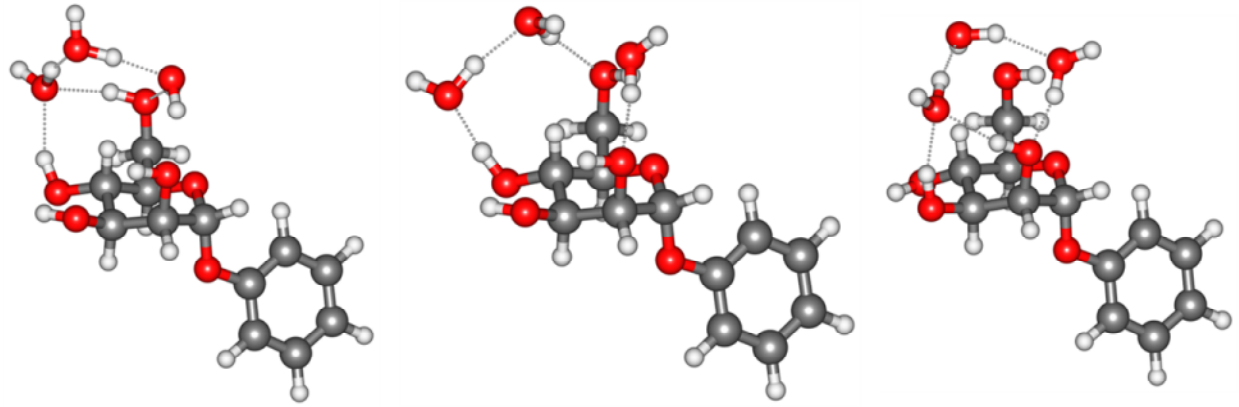


Figure S1. Experimental IRID spectrum of (exp) α-PhMan•$(D_2O)_2$ complex and calculated vibrational (stick) spectra of (a – f) various conformers A – F, respectively, associated with the complex.

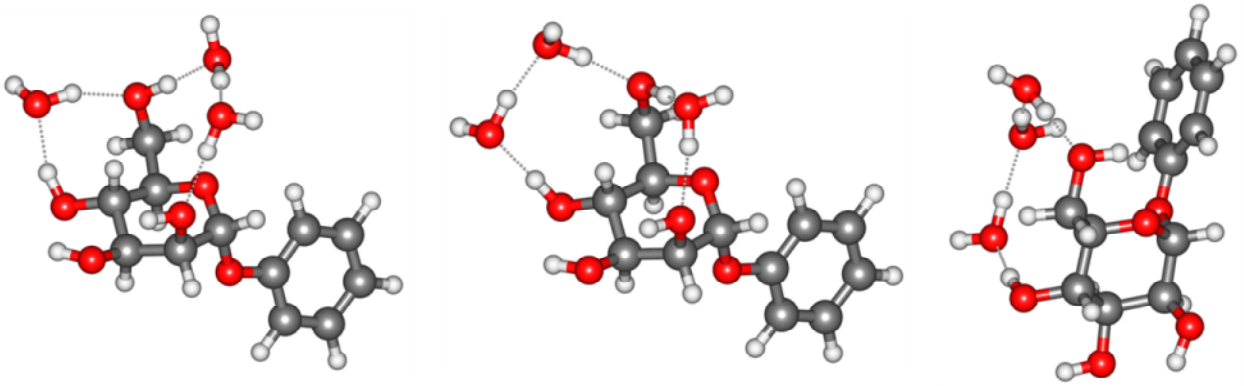
4. α-PhMan•$(D_2O)_3$

(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	6.44	4.91
C	8.99	5.79
D	5.05	6.06
E	5.97	7.56
F	15.33	8.21



A B C



D E F

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

A			
6	-0.881529	0.579628	0.762694
6	0.082820	1.772493	0.752531
6	0.843319	1.843073	-0.574237
6	1.488645	0.494955	-0.889642
6	0.412598	-0.605771	-0.897860
8	-0.251829	-0.620777	0.385095
8	0.988670	1.583561	1.845102
8	1.830445	2.863225	-0.427535
8	2.165595	0.613191	-2.139166
6	0.950511	-2.016856	-1.124829
8	1.994265	-2.386602	-0.223352
1	1.718720	2.214016	1.705972
1	2.450355	2.763063	-1.170912
1	2.850597	-2.116848	-0.615745
1	-1.250804	0.404118	1.778333
1	-0.490736	2.694890	0.905759
1	0.143072	2.108658	-1.378745
1	2.211353	0.271311	-0.099857
1	-0.322229	-0.394346	-1.688308
1	2.992947	0.094811	-2.072898
1	1.291725	-2.102400	-2.163849
1	0.131059	-2.726050	-0.973006
8	-1.950928	0.934825	-0.098671
6	-5.479978	0.236459	-0.651582
6	-4.227061	0.846394	-0.679296
6	-3.148490	0.250634	-0.013687
6	-3.318388	-0.958165	0.670420
6	-4.585638	-1.552863	0.696022
6	-5.668596	-0.965719	0.040328
1	-6.313316	0.705948	-1.168210
1	-4.066330	1.783856	-1.203696
1	-2.480042	-1.445885	1.153976
1	-4.714992	-2.491361	1.229284
1	-6.646513	-1.438473	0.063289
8	4.287500	-1.099857	-1.277456
1	4.648112	-0.789048	-0.398803
1	5.026743	-1.484104	-1.772033
8	4.831296	-0.278937	1.223592
1	5.551684	-0.589656	1.791245
1	3.977666	-0.512172	1.691964
8	2.426463	-0.954487	2.225750
1	1.826851	-0.180309	2.212218
1	2.082986	-1.548723	1.521991

B			
6	-0.878715	0.347276	0.870262
6	0.109816	1.474525	1.186627
6	0.912011	1.857482	-0.056911
6	1.540998	0.625574	-0.714891
6	0.458547	-0.429562	-1.000838
8	-0.264167	-0.736130	0.217339
8	0.989009	1.003132	2.220179
8	1.914086	2.774444	0.385672
8	2.180355	1.026238	-1.917721
6	0.998604	-1.769224	-1.488163
8	1.896313	-2.384631	-0.564065
1	1.734110	1.633059	2.235906
1	2.565318	2.864160	-0.331896
1	1.549776	-2.294103	0.345669
1	-1.289867	-0.069634	1.795897
1	-0.448849	2.341061	1.559885
1	0.245590	2.346244	-0.780639
1	2.275641	0.197702	-0.024419
1	-0.239043	-0.041023	-1.755623
1	3.146251	0.847228	-1.828009
1	0.150687	-2.438661	-1.687647
1	1.553854	-1.620777	-2.417648
8	-1.906916	0.942905	0.098778
6	-4.630561	-1.575768	0.152435
6	-3.346823	-1.038995	0.308416
6	-3.126237	0.302425	-0.022300
6	-4.169950	1.091235	-0.521298
6	-5.439728	0.538752	-0.679577
6	-5.679501	-0.797714	-0.339148
1	-4.799749	-2.618283	0.410141
1	-2.533728	-1.666764	0.653692
1	-3.969480	2.128663	-0.772490
1	-6.246098	1.157286	-1.065309
1	-6.670475	-1.225937	-0.461022
8	4.798707	0.602824	-1.204310
1	5.544963	0.500904	-1.812677
1	4.795415	-0.203269	-0.620699
8	4.447002	-1.634955	0.289592
1	3.686181	-2.027695	-0.193667
1	4.063637	-1.484052	1.174339
8	2.258086	-1.525042	2.230228
1	2.152996	-1.946076	3.096494
1	1.742289	-0.686360	2.266506

C			
6	-0.652595	-0.197204	-0.764458
6	0.456154	-1.220574	-1.054328
6	0.984288	-1.770461	0.279911
6	1.423906	-0.636310	1.207918
6	0.351540	0.452514	1.352818
8	-0.193075	0.837710	0.071927
8	1.430231	-0.510396	-1.830843
8	2.024249	-2.734862	0.140559
8	1.694519	-1.128165	2.518865
6	0.915817	1.739877	1.953493
8	1.989014	2.281936	1.185798
1	2.308750	-0.946019	-1.795462
1	2.832131	-2.298379	-0.203820
1	1.680056	2.448421	0.273040
1	-0.962643	0.301082	-1.689549
1	0.044263	-2.043188	-1.651590
1	0.156413	-2.310090	0.751426
1	2.328334	-0.175165	0.793529
1	-0.453780	0.073747	1.996495
1	2.203555	-1.950340	2.414700
1	0.105112	2.475090	2.051671
1	1.318955	1.526322	2.946460
8	-1.737940	-0.920111	-0.213419
6	-5.363316	-0.760450	0.076882
6	-4.054121	-1.237425	0.043087
6	-2.997787	-0.351404	-0.201482
6	-3.247290	1.010717	-0.402749
6	-4.568941	1.471926	-0.374588
6	-5.629748	0.597247	-0.136097
1	-6.178923	-1.453869	0.265528
1	-3.831432	-2.289015	0.198228
1	-2.430694	1.707926	-0.549779
1	-4.760325	2.530763	-0.530189
1	-6.651068	0.966832	-0.110811
8	4.370961	1.352279	-0.273654
1	3.898087	1.562798	0.556015
1	3.816169	1.805296	-0.944687
8	4.051199	-1.188956	-1.125887
1	4.277733	-0.282685	-0.765102
1	4.849258	-1.540878	-1.547694
8	2.132018	2.180471	-1.723372
1	1.751683	1.272688	-1.813157
1	1.901511	2.668688	-2.527482

D			
6	0.649115	-0.412172	0.845468
6	-0.276442	-1.530103	1.349861
6	-1.136992	-2.089525	0.214701
6	-1.799479	-0.972179	-0.590549
6	-0.713878	-0.009208	-1.100395
8	-0.016104	0.531629	0.045508
8	-1.110891	-0.977704	2.376745
8	-2.119101	-2.929862	0.822878
8	-2.534391	-1.597131	-1.634799
6	-1.230913	1.173008	-1.916997
8	-2.328987	1.865757	-1.335378
1	-1.881941	-1.572118	2.446392
1	-2.797933	-3.092651	0.143611
1	-2.045479	2.392382	-0.543908
1	1.048472	0.156439	1.692406
1	0.339415	-2.327382	1.782769
1	-0.501153	-2.682027	-0.458054
1	-2.476330	-0.411538	0.065738
1	-0.000748	-0.558176	-1.732376
1	-3.330261	-1.045853	-1.816775
1	-1.577762	0.795915	-2.884099
1	-0.395986	1.862578	-2.097913
8	1.703818	-1.070503	0.160818
6	5.196605	-0.601162	-0.749385
6	3.962377	-1.189948	-0.479871
6	2.882085	-0.391129	-0.084592
6	3.030945	0.995519	0.032264
6	4.280059	1.569550	-0.233703
6	5.364690	0.782897	-0.623823
1	6.031392	-1.227508	-1.053609
1	3.817607	-2.263071	-0.564155
1	2.188772	1.625085	0.294918
1	4.392918	2.647038	-0.143186
1	6.327860	1.240202	-0.832509
8	-4.524515	0.325424	-1.757546
1	-3.873120	1.049903	-1.584300
1	-5.045420	0.593411	-2.528104
8	-1.704701	3.366652	0.858324
1	-1.656753	2.776980	1.650917
1	-2.415424	3.998083	1.044527
8	-1.707899	1.670616	3.033250
1	-1.485046	0.749668	2.765744
1	-1.169935	1.860336	3.815693

E			
6	-0.977809	0.456167	0.887676
6	-0.062127	1.653483	1.159793
6	0.794574	1.955827	-0.066430
6	1.534785	0.710934	-0.561074
6	0.550541	-0.457648	-0.765028
8	-0.264161	-0.657875	0.416505
8	0.761238	1.308114	2.283982
8	1.717471	2.974374	0.322398
8	2.173313	1.052277	-1.782401
6	1.225574	-1.801946	-1.014207
8	2.157294	-2.176620	-0.001132
1	1.488159	1.957507	2.298378
1	2.370805	3.052710	-0.394731
1	1.837490	-1.946330	0.902970
1	-1.453764	0.122051	1.816119
1	-0.677316	2.524336	1.416314
1	0.144898	2.322656	-0.872739
1	2.279352	0.424290	0.191162
1	-0.097650	-0.230968	-1.622696
1	3.124619	0.787935	-1.752201
1	1.782547	-1.755946	-1.954405
1	0.446345	-2.570486	-1.108952
8	-1.958320	0.915617	-0.026734
6	-5.400548	0.267618	-1.018301
6	-4.170041	0.893147	-0.825136
6	-3.138184	0.210099	-0.169777
6	-3.331278	-1.099589	0.283386
6	-4.576392	-1.709954	0.089720
6	-5.613323	-1.036972	-0.557655
1	-6.197882	0.804486	-1.525901
1	-3.991775	1.908082	-1.168163
1	-2.523823	-1.649528	0.752550
1	-4.724033	-2.727728	0.442273
1	-6.573845	-1.522167	-0.706933
8	1.893212	-1.289439	2.625548
1	1.439725	-0.419652	2.555474
1	1.414391	-1.786146	3.305311
8	4.868866	-1.959187	-0.271679
1	5.249138	-1.973197	0.619167
1	3.896547	-2.109549	-0.153677
8	4.835926	0.414675	-1.586512
1	4.958873	-0.449020	-1.111931
1	5.313860	0.334168	-2.424995

F			
6	0.456397	-1.660932	-0.549905
6	1.792612	-2.056428	0.092805
6	2.446986	-0.837111	0.749844
6	2.519629	0.352596	-0.214059
6	1.131358	0.645068	-0.805033
8	0.568019	-0.544909	-1.401858
8	2.610717	-2.592521	-0.936591
8	3.758854	-1.239407	1.150734
8	3.076951	1.490534	0.430651
6	1.181895	1.671522	-1.926845
8	-0.125791	1.943733	-2.455355
1	3.517619	-2.609715	-0.583525
1	4.255568	-0.427333	1.352645
1	-0.521616	1.089315	-2.699108
1	0.087318	-2.473448	-1.183027
1	1.591242	-2.819924	0.857472
1	1.858641	-0.547461	1.631180
1	3.206570	0.100145	-1.029520
1	0.455735	0.999738	-0.015994
1	2.471966	1.768336	1.159819
1	1.834907	1.312632	-2.733075
1	1.571010	2.619292	-1.551101
8	-0.429043	-1.423709	0.537854
6	-3.932753	-0.957346	1.385519
6	-2.548812	-1.101316	1.483550
6	-1.780468	-1.287631	0.324226
6	-2.399862	-1.325946	-0.930416
6	-3.790519	-1.186398	-1.010244
6	-4.563106	-0.998417	0.136570
1	-4.519956	-0.819649	2.289930
1	-2.046692	-1.099222	2.447488
1	-1.817428	-1.451672	-1.835673
1	-4.266780	-1.218206	-1.986962
1	-5.640689	-0.885487	0.060671
8	-1.833816	3.336070	-0.779766
1	-1.240701	2.897775	-1.435613
1	-1.850219	4.279033	-0.997907
8	-1.392808	2.289359	1.730580
1	-1.910439	1.467672	1.719901
1	-1.577201	2.731157	0.866316
8	1.238033	2.072526	2.457367
1	1.413544	2.718244	3.157384
1	0.278536	2.169407	2.223684

(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}
ν1	26.6422	0.3336	22.3611	0.0412	29.0542	0.3546
ν2	36.3010	0.2910	30.8810	0.9556	41.7365	0.0968
ν3	46.1289	0.3680	38.0010	0.2497	44.3020	0.2508
ν4	50.0950	2.0609	45.4249	0.7318	65.1893	1.5971
ν5	63.8264	0.6364	61.0054	1.3974	76.5444	1.7453
ν6	87.8309	0.4193	74.1838	0.6576	89.9504	0.3151
ν7	104.8956	0.8970	76.3582	0.0958	94.9610	3.7278
ν8	118.2882	2.8581	101.9103	0.7363	100.8620	2.3092
ν9	123.2039	1.7597	107.3108	2.6187	119.8164	1.0204
ν10	125.5424	2.1512	118.0157	1.0995	134.0094	4.0140
ν11	154.6245	3.3295	136.2643	5.4613	138.0449	5.6524
ν12	165.2940	3.6944	157.4619	3.0245	169.8469	3.9526
ν13	169.7396	6.7868	184.2051	12.2680	175.4267	24.1935
ν14	200.7027	14.1184	192.4001	54.6341	180.6478	4.6737
ν15	210.6467	17.9494	195.5638	7.0301	194.9401	8.6839
ν16	213.2729	6.5831	206.9434	0.8197	209.1272	32.6059
ν17	221.6673	7.3700	215.6630	8.0524	216.1740	10.5353
ν18	242.7675	43.4474	229.1035	25.9038	217.3312	2.4423
ν19	254.2548	10.8117	237.9888	23.5332	237.5267	23.2981
ν20	260.1007	1.9976	246.5525	46.7314	248.9970	4.3959
ν21	262.3956	35.2864	258.4812	1.3956	263.8049	26.2090
ν22	268.7973	28.2285	264.1128	4.0516	276.3139	21.3166
ν23	278.7841	3.8641	275.8279	13.7202	283.6350	20.1928
ν24	298.9231	38.0041	278.9624	13.6846	288.1989	3.6726
ν25	328.4582	4.3340	297.2796	14.1847	306.4482	0.3555
ν26	345.5687	29.2379	320.7583	1.7118	336.7914	1.1721
ν27	364.0051	2.8581	328.4214	1.0928	345.8213	31.1479
ν28	399.1111	22.2561	358.0812	25.4992	364.4262	24.6497
ν29	404.5986	4.8005	371.2092	36.4740	372.8661	37.6744
ν30	422.8638	0.4193	414.1647	39.1900	384.0632	46.5384
ν31	426.9834	12.2421	419.8992	53.4181	418.0744	25.1942
ν32	432.5045	48.9482	421.6897	0.8820	423.1886	0.2192
ν33	447.4733	82.0534	431.0863	60.6530	424.9276	34.8439
ν34	466.5551	66.2996	442.1772	33.0121	443.9379	0.7527
ν35	483.5294	35.9818	469.7353	69.5927	479.5662	5.3412
ν36	509.8360	2.9170	486.2689	64.9316	502.0740	22.6700
ν37	510.2538	60.8991	506.7885	1.6868	519.9106	7.2212
ν38	521.9989	4.4535	520.2853	7.2314	533.7707	99.6269
ν39	574.0258	47.9248	555.3029	75.4635	581.8336	8.1326
ν40	588.4087	103.3405	576.6520	21.6460	590.3365	112.4946
ν41	595.1246	52.9857	610.2639	30.2323	619.2560	6.1419
ν42	617.8040	1.5657	621.2137	12.3643	636.9750	11.1007
ν43	639.5273	5.8805	633.5803	102.2455	651.3912	37.5608
ν44	672.4263	19.9859	642.8265	101.5484	672.2024	93.5388
ν45	689.0083	19.9008	675.2794	10.6364	681.4655	56.1972
ν46	698.1404	53.5006	683.2621	40.1169	698.5483	55.3111
ν47	699.4125	20.3650	687.1751	28.2142	699.9044	66.5273
ν48	732.8225	214.0190	698.1351	19.5762	730.4627	209.7946
ν49	764.6400	69.3792	764.7012	71.5166	762.4904	16.5989
ν50	800.9061	17.1800	779.9936	135.7726	765.3132	71.6775
ν51	810.9303	21.1338	812.2565	17.3675	809.5044	20.3011
ν52	836.8628	1.2989	836.8889	0.8332	838.1071	0.7830
ν53	842.5108	2.5213	847.1353	17.5347	849.9066	32.6040
ν54	854.9190	24.9849	860.3423	14.5323	859.8614	15.8640
ν55	890.8793	17.7803	890.7204	12.5706	890.5114	11.3997
ν56	906.4234	7.3196	906.5156	6.7401	907.2352	5.2332
ν57	925.2696	12.3340	923.6871	10.7628	920.1445	11.6084
ν58	970.8955	0.6658	971.2547	0.4901	971.2144	0.2537
ν59	991.0557	15.6047	992.2903	0.7440	991.6940	1.2669
ν60	993.8444	98.7980	999.8361	121.0554	995.5023	28.1986
ν61	1013.1790	19.5650	1013.4630	18.7602	1013.8721	11.7497
ν62	1033.6287	265.7905	1030.5607	252.6585	1026.4879	215.7529
ν63	1049.4660	21.3789	1045.3148	30.0620	1043.4845	85.9788
ν64	1057.1008	158.9735	1058.3522	43.5627	1052.1357	4.1528
ν65	1060.8944	121.9315	1060.1138	264.3623	1063.6185	304.3222
ν66	1090.8704	115.8513	1092.7266	88.3394	1095.3964	130.8113
ν67	1098.9171	65.0651	1101.8571	74.7923	1105.5309	45.0128
ν68	1110.5070	23.4893	1109.8227	27.9910	1109.9078	25.7279
ν69	1115.7761	6.4862	1116.8644	2.2608	1119.0597	8.8520
ν70	1127.9613	92.1577	1131.2667	44.6303	1119.7975	64.3670
ν71	1138.5751	56.1805	1134.6717	123.3602	1132.3741	106.6081
ν72	1148.0090	10.0743	1142.0121	34.3506	1163.1114	85.8614
ν73	1187.5670	2.5565	1187.8198	2.4186	1187.8264	2.4377
ν74	1206.2275	12.8647	1205.9960	10.6623	1206.7019	9.7628
ν75	1229.9648	53.8933	1232.8596	44.6366	1233.4348	37.2767

v76	1242.7007	40.4465	1240.8694	35.3654	1237.4761	21.5350
v77	1252.9046	60.3369	1245.9891	70.9745	1245.4133	63.3877
v78	1256.8668	237.3268	1251.2982	45.6203	1254.1527	66.1293
v79	1260.1121	83.3228	1258.1356	229.6445	1259.0453	257.3855
v80	1264.1366	38.5277	1267.5527	46.8845	1279.4077	71.9541
v81	1274.5360	56.0131	1277.8269	40.5038	1291.3232	41.8534
v82	1288.9514	1.0899	1298.4262	75.0818	1303.8385	3.4419
v83	1323.4704	9.7497	1324.7582	4.8125	1326.1275	8.1770
v84	1340.5253	7.1546	1339.6504	4.9204	1340.8834	3.4867
v85	1350.3851	1.8439	1346.5878	2.1091	1342.6208	2.6061
v86	1361.3999	12.4789	1359.0933	20.5871	1355.8917	11.6540
v87	1367.8382	9.3866	1367.2014	9.9396	1366.2173	6.4997
v88	1384.2412	26.3453	1374.8622	6.8360	1371.7243	38.7865
v89	1400.1481	18.5979	1389.1772	31.2181	1390.2076	15.8042
v90	1410.1875	2.4508	1400.7818	13.8789	1397.2200	11.9324
v91	1418.1352	24.8990	1419.3350	0.9138	1412.5565	14.6490
v92	1425.0101	10.0912	1424.2014	20.5412	1426.3998	36.1977
v93	1428.7799	35.7910	1433.7545	36.2391	1433.7334	24.9821
v94	1444.9619	17.9539	1445.3548	64.2615	1440.2742	20.4414
v95	1467.6983	49.7847	1449.3997	5.3187	1455.5882	11.3646
v96	1477.9826	1.0143	1498.1771	1.0037	1484.9515	43.7771
v97	1498.2997	1.0518	1498.3877	28.2813	1498.1223	1.3005
v98	1510.5959	7.5840	1518.1360	5.3112	1512.4987	5.5985
v99	1535.9427	108.6005	1535.6042	107.1386	1536.0589	107.5770
v100	1638.3092	25.4225	1638.4135	25.4136	1638.4643	24.4084
v101	1652.2562	70.6241	1652.0031	67.7831	1652.3004	70.0240
v102	2307.0636	427.8416	2404.0068	369.5600	2327.9981	404.8322
v103	2381.0941	539.4732	2539.3497	277.4604	2500.1955	327.9082
v104	2564.9895	157.1649	2575.4251	208.0363	2590.8769	136.9893
v105	2665.0758	187.5819	2699.6748	93.2413	2687.0881	109.7883
v106	2778.3121	55.0931	2782.7799	77.8974	2781.0118	67.1572
v107	2781.8180	65.8226	2783.7591	62.1600	2787.5445	78.8817
v108	3033.2567	4.9790	3038.6146	26.1705	3037.8506	36.1370
v109	3041.7982	19.6704	3047.8701	2.5344	3055.1271	24.4351
v110	3062.6398	43.9285	3052.7335	48.5929	3065.0820	28.8060
v111	3066.2839	38.6872	3070.7724	33.5019	3071.3364	19.7370
v112	3095.8146	19.2100	3088.7618	13.8421	3083.9264	27.7442
v113	3104.7396	15.9094	3089.2967	32.3741	3099.0661	31.7271
v114	3117.5556	25.0124	3133.7799	14.4154	3136.8217	12.7233
v115	3183.3971	1.1571	3184.1078	1.0963	3183.7464	1.2384
v116	3191.4505	14.3016	3192.2537	13.6869	3191.8220	14.3439
v117	3205.7004	26.9655	3206.1231	26.2162	3206.2431	26.7493
v118	3212.9112	10.8978	3213.7001	10.2960	3213.8918	9.7924
v119	3234.4317	1.3372	3233.1966	1.8593	3234.8852	1.7114
v120	3566.3956	169.8172	3441.9286	859.9666	3533.2554	82.5153
v121	3607.5467	647.4882	3643.1828	133.8047	3577.1504	721.6786
v122	3693.0441	78.5415	3673.1587	88.2466	3631.9858	168.4162
v123	3714.9413	52.7124	3715.7979	59.9313	3716.6385	47.3694

	D		E		F	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
ν1	23.2505	0.0393	17.6836	0.7571	29.6659	0.0748
ν2	29.9910	0.5178	27.7720	0.1995	33.7585	0.1335
ν3	34.5951	2.2097	35.2625	0.7874	36.8207	1.1494
ν4	45.1207	0.1130	35.9340	0.6396	44.9798	0.1082
ν5	50.5248	1.7999	47.1590	0.4952	54.2701	0.9311
ν6	53.8875	1.2108	49.5253	1.2803	62.4565	0.9347
ν7	71.7280	0.1669	76.5181	0.0154	64.4526	1.8770
ν8	99.2374	1.1554	100.9723	0.4570	67.3164	1.3807
ν9	106.4582	1.4792	106.6661	3.7127	93.1397	1.1961
ν10	113.6397	2.6212	120.7242	7.7525	111.5791	3.8626
ν11	135.2664	16.9725	133.1075	8.3052	119.5709	3.3341
ν12	154.3517	37.0997	166.6723	1.6143	137.1746	16.7016
ν13	174.1096	9.0986	178.0490	12.9838	139.8223	47.5772
ν14	178.7083	14.7443	183.2527	40.9533	166.0073	36.6003
ν15	189.9391	36.7882	189.2467	45.9668	174.2252	5.2226
ν16	194.8864	32.7364	202.6397	25.8792	193.2200	3.5378
ν17	211.4907	2.1232	206.2751	10.9414	208.6481	3.7314
ν18	223.8378	40.7687	222.0628	18.2521	218.3392	7.5278
ν19	232.2994	56.7446	234.9851	29.2158	233.2160	6.6842
ν20	256.8833	10.2919	252.7120	12.2459	252.2417	34.7823
ν21	257.3424	18.4372	255.3413	60.1625	255.8118	47.4529
ν22	266.9866	11.6128	258.9493	15.1079	259.2657	18.1396
ν23	282.0470	31.6376	267.0122	9.3941	268.1721	52.9933
ν24	291.3215	9.7243	283.2316	22.7326	290.8721	14.3980
ν25	301.3416	29.4164	284.9962	32.2648	297.4550	20.2895
ν26	304.8277	28.7787	298.3184	37.7632	306.3001	3.3421
ν27	327.6889	7.8846	329.7329	2.4790	320.1179	8.2485
ν28	340.6804	24.1307	353.9487	15.5357	356.6172	2.1250
ν29	358.2580	14.2153	369.9686	2.5609	361.1849	1.7180
ν30	370.1607	6.1814	379.6545	13.7940	376.7774	23.0293
ν31	413.6571	11.8571	422.4173	0.4326	399.7141	10.9258
ν32	423.1292	0.0121	427.6339	13.3566	419.3131	28.6769
ν33	433.6565	7.1053	435.8482	34.7283	423.7770	0.4944
ν34	470.4959	47.1125	447.6275	72.1384	439.8839	33.7488
ν35	483.5153	35.1783	469.8271	84.4307	441.2385	119.4906
ν36	499.5097	144.7351	483.5197	78.9992	464.9187	78.0283
ν37	510.0071	7.2556	506.1729	2.0168	475.1260	95.2111
ν38	521.2630	6.2116	520.2876	10.0528	517.1499	10.6631
ν39	565.5327	40.4046	550.6621	87.0195	532.6030	2.3130
ν40	581.1016	63.3998	556.3258	16.8472	559.3926	20.3303
ν41	588.1249	28.6478	584.5134	17.8993	566.8148	70.4764
ν42	613.1717	30.2230	618.6167	5.9582	600.8262	34.7350
ν43	619.3924	4.5558	638.9602	14.0448	604.2995	17.5981
ν44	643.1307	10.9231	672.2434	23.6059	624.4335	1.2656
ν45	680.3473	6.2954	681.1207	42.1110	659.0844	70.4879
ν46	690.7929	38.5751	686.0209	18.9728	662.4471	45.5369
ν47	699.4146	21.5943	698.6867	19.8069	690.5930	11.4902
ν48	765.0945	70.8306	765.4908	69.4425	699.3826	15.5157
ν49	784.8808	98.2998	782.3119	90.5468	762.3927	73.8968
ν50	813.8295	21.5706	799.5953	152.5229	795.1276	104.2222
ν51	833.6326	21.1811	815.8543	36.5784	804.7465	43.6858
ν52	838.9306	1.0988	837.6843	0.7096	829.8926	16.6858
ν53	851.7108	44.7194	844.1314	9.9558	840.0316	6.3977
ν54	872.6026	102.1077	858.6808	13.2686	850.3998	19.7742
ν55	891.8738	14.1301	891.1040	14.1583	891.7810	10.6607
ν56	908.2881	6.2755	907.5064	6.5380	903.2332	8.1417
ν57	931.1033	8.9284	926.0968	9.0039	972.5968	7.0063
ν58	971.5143	0.6197	971.7477	0.5738	976.8626	58.8789
ν59	991.2918	4.2070	992.3294	1.3317	993.2124	0.9414
ν60	996.7191	131.9901	999.1026	115.4417	1010.6984	35.9870
ν61	1013.0298	19.8250	1013.5310	19.3083	1021.4164	107.9707
ν62	1033.1423	307.2275	1033.3018	273.2337	1026.0176	229.0736
ν63	1051.3036	43.1465	1047.2333	17.2132	1050.2812	26.6817
ν64	1060.3205	58.9357	1060.2043	222.1408	1061.9422	35.3295
ν65	1064.1348	125.1520	1062.1973	59.9398	1062.9476	70.2585
ν66	1094.7907	113.3265	1093.0061	100.8678	1085.2393	97.1632
ν67	1101.4849	68.3128	1103.3639	72.5430	1105.3986	118.8712
ν68	1110.4415	25.8790	1110.0795	25.5823	1109.5997	44.6245
ν69	1113.0600	0.5603	1115.9239	2.8909	1120.2737	5.7016
ν70	1135.7360	110.1299	1130.5341	42.6423	1127.9392	76.2818
ν71	1139.7710	47.5710	1136.7970	123.7011	1135.5985	67.7427
ν72	1154.6101	22.9820	1147.0926	12.0258	1148.8766	34.8398
ν73	1187.4674	2.4202	1187.9469	2.4239	1188.0558	2.3909
ν74	1206.3274	10.9905	1205.8430	12.1355	1204.2251	15.4649
ν75	1231.6143	62.3928	1230.8036	58.0499	1225.0669	11.5068

v76	1237.4831	45.2694	1239.7868	82.4909	1239.4817	39.9376
v77	1241.5074	40.8697	1250.3543	20.2900	1242.9900	43.2388
v78	1257.5500	260.0304	1255.4771	102.0339	1247.1157	40.3087
v79	1261.2866	37.8061	1258.9463	91.5322	1263.4804	62.2955
v80	1269.0761	12.3640	1263.5390	92.2527	1265.9928	41.7680
v81	1271.2370	54.1000	1269.4205	20.2684	1268.6679	209.2433
v82	1290.2480	28.5650	1287.0343	43.1551	1281.5892	15.8856
v83	1326.0671	5.3002	1319.0164	15.2740	1302.2286	11.5219
v84	1339.6807	4.1029	1337.6087	3.4823	1335.5868	4.5576
v85	1352.1160	3.3133	1347.6663	2.0513	1349.2020	10.3728
v86	1365.8404	12.5401	1357.2745	27.8035	1357.0073	11.3602
v87	1367.8461	6.5285	1367.3388	10.8014	1366.7385	11.7077
v88	1387.0716	32.1276	1375.8709	14.6742	1379.6230	23.3839
v89	1397.4337	13.0456	1385.4451	23.2629	1392.4703	10.3995
v90	1406.6367	6.2747	1404.3168	11.6053	1401.8628	16.6237
v91	1417.3173	1.3301	1416.5492	2.1121	1408.9007	11.6489
v92	1427.0149	17.7787	1424.1146	19.8810	1421.1403	17.8029
v93	1432.7901	68.1146	1428.8190	48.5020	1435.9949	49.1397
v94	1447.7758	24.0976	1445.7893	42.0587	1446.2773	8.5925
v95	1480.7965	57.6491	1454.8262	47.4295	1448.3653	24.5522
v96	1490.6624	30.7088	1496.1298	24.1692	1496.9852	43.6931
v97	1498.0202	1.5324	1498.2974	1.3968	1497.6618	10.4174
v98	1505.5635	12.2894	1515.6900	6.1980	1516.2288	2.8295
v99	1535.9558	104.7005	1536.4444	107.5998	1535.5715	104.5185
v100	1638.0584	24.0150	1638.7304	25.0156	1637.0467	23.7702
v101	1652.1038	67.6962	1652.4008	69.0172	1650.7233	73.9826
v102	2476.6759	288.3153	2418.7573	367.4582	2437.0306	424.1139
v103	2488.8324	391.4102	2483.3833	489.2752	2494.9362	338.9633
v104	2554.5826	279.2679	2561.4891	218.9411	2528.9164	222.5639
v105	2779.9862	56.5425	2779.4362	71.4704	2750.1704	104.6606
v106	2786.0371	86.8532	2780.8364	55.3881	2784.1382	59.8775
v107	2786.9452	71.6842	2785.9837	75.7292	2789.7159	80.0277
v108	3032.4373	3.1895	3039.2218	27.0577	3034.2817	29.1497
v109	3041.2649	9.2019	3047.2932	6.8230	3050.2756	33.9029
v110	3052.8249	50.8486	3052.1230	32.8873	3052.1099	0.1110
v111	3067.7533	14.8812	3069.0016	22.9802	3063.1489	6.7481
v112	3071.0118	52.8696	3074.3566	46.0132	3085.4193	50.1924
v113	3086.0082	25.7474	3085.4756	26.6199	3102.4887	23.1231
v114	3112.8305	30.6791	3120.1696	21.6086	3156.4909	8.8982
v115	3183.2168	0.9423	3183.6446	1.1147	3185.1801	2.3657
v116	3191.3190	14.1856	3191.7487	14.2613	3191.7839	9.0456
v117	3205.3832	26.2838	3206.0575	27.0631	3203.2881	14.4314
v118	3212.7913	10.9410	3213.6988	9.5975	3212.7936	17.8458
v119	3233.5049	0.9588	3232.5989	1.8469	3230.0816	4.1174
v120	3355.8656	868.7938	3415.3084	1071.6834	3448.3787	477.5903
v121	3475.5460	681.4418	3472.3948	485.1708	3705.7185	74.8581
v122	3667.7908	105.1409	3689.3774	85.3061	3712.7561	44.8923
v123	3702.3777	59.0692	3713.2446	54.7765	3727.5858	45.4461

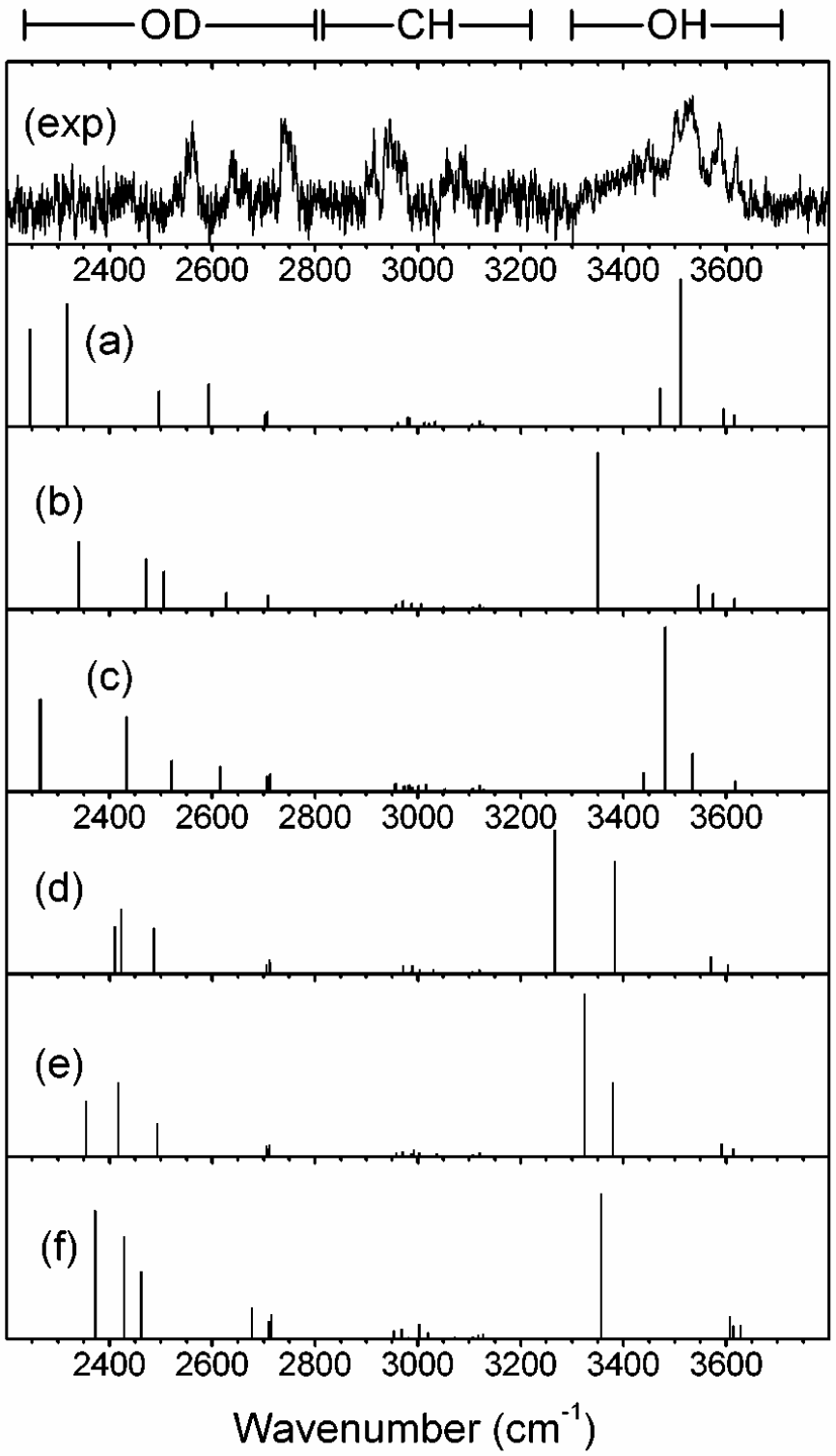
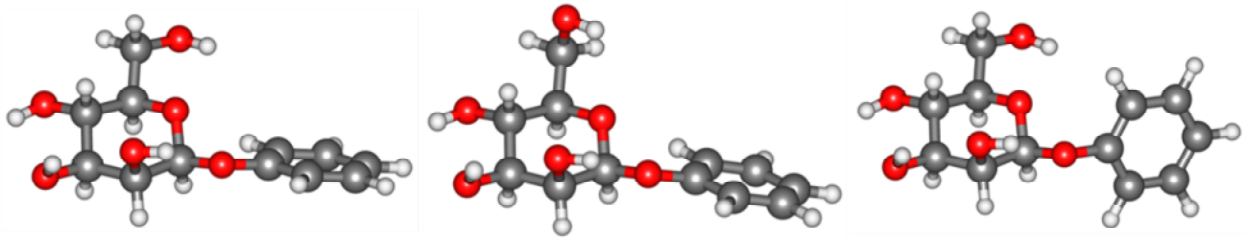


Figure S2. Experimental IRID spectrum of (exp) α-PhMan•$(D_2O)_3$ complex and calculated vibrational (stick) spectra of (a – f) various conformers A – F, respectively, associated with the complex.

5. β-PhMan

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

Conformer	B3LYP/6-311++G(d,p) energy / kJ mol^{-1}	MP2/6-311++G(d,p)//B3LYP/6-311++G(d,p) energy / kJ mol^{-1}
A	0.00	0.00
B	1.41	1.32
C	4.02	1.45



A B C

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

A			
6	-0.060427	-0.583722	-0.337962
6	-1.150565	-1.661531	-0.252379
6	-2.499203	-1.071776	-0.670144
6	-2.787662	0.243217	0.065248
6	-1.614868	1.210653	-0.111753
8	-0.412492	0.585770	0.370114
8	-1.311448	-2.154681	1.071113
8	-3.560231	-2.000140	-0.476265
8	-3.956250	0.860697	-0.457744
6	-1.770630	2.503486	0.676383
8	-0.664676	3.374684	0.487607
1	-0.438349	-2.346657	1.433321
1	-3.411524	-2.429223	0.377350
1	0.120449	2.917100	0.808823
1	-0.877812	-2.479902	-0.931622
1	-2.481403	-0.860065	-1.744404
1	-2.908012	0.031404	1.135900
1	-1.498780	1.455350	-1.178170
1	-4.643867	0.184290	-0.495485
1	-2.657618	3.030951	0.326831
1	-1.904512	2.261314	1.739022
8	1.087197	-1.129956	0.251775
1	0.130806	-0.338991	-1.395367
6	4.909842	0.431778	-0.329336
6	3.811725	1.153769	-0.786712
6	2.512515	0.675332	-0.605651
6	2.323980	-0.550262	0.032323
6	3.417647	-1.281966	0.497507
6	4.704440	-0.787805	0.317406
1	5.913503	0.814824	-0.469795
1	3.955976	2.106983	-1.282702
1	1.669947	1.265924	-0.937794
1	3.243594	-2.230682	0.990868
1	5.550039	-1.360657	0.680842

B			
6	0.050082	-0.528977	-0.327132
6	-0.993815	-1.637482	-0.136613
6	-2.338356	-1.190658	-0.708190
6	-2.739156	0.190575	-0.179748
6	-1.610312	1.201463	-0.404899
8	-0.387797	0.716340	0.178024
8	-1.207273	-1.938142	1.235978
8	-3.360743	-2.147389	-0.451843
8	-3.881392	0.674698	-0.877505
6	-1.870372	2.558229	0.242154
8	-1.971257	2.474350	1.655110
1	-0.348806	-2.062051	1.657645
1	-3.259102	-2.433813	0.465864
1	-1.160580	2.064895	1.979613
1	-0.642968	-2.530179	-0.671015
1	-2.259441	-1.127018	-1.798711
1	-2.941304	0.126715	0.895169
1	-1.477950	1.347886	-1.488248
1	-4.560105	-0.008906	-0.825599
1	-1.069085	3.248074	-0.053450
1	-2.820769	2.948683	-0.122207
8	1.185496	-0.925673	0.393225
1	0.295026	-0.431474	-1.397166
6	4.999679	0.555364	-0.407202
6	4.807501	-0.617276	0.324663
6	3.523724	-1.088803	0.575164
6	2.421415	-0.379559	0.096198
6	2.596758	0.802080	-0.622639
6	3.892341	1.256313	-0.875679
1	6.000933	0.919456	-0.604137
1	5.660689	-1.172510	0.697593
1	3.359053	-2.003085	1.132628
1	1.743077	1.376997	-0.953494
1	4.028125	2.175241	-1.434858

C			
6	-0.092559	-0.720341	-0.285275
6	-1.279816	-1.666080	-0.054375
6	-2.576877	-1.007733	-0.529130
6	-2.719312	0.416222	0.022693
6	-1.465375	1.227789	-0.311168
8	-0.320014	0.564716	0.253201
8	-1.453854	-1.971396	1.323181
8	-3.715552	-1.794111	-0.195825
8	-3.842052	1.065376	-0.559074
6	-1.471007	2.635428	0.264794
8	-0.305920	3.358915	-0.104257
1	-0.591018	-2.193014	1.693916
1	-3.582456	-2.120743	0.704467
1	0.456501	2.836223	0.169890
1	-1.101455	-2.586709	-0.625701
1	-2.568417	-0.944817	-1.622357
1	-2.823581	0.366063	1.114607
1	-1.349719	1.292502	-1.403287
1	-4.588139	0.456262	-0.494596
1	-2.326797	3.182084	-0.130258
1	-1.568952	2.574618	1.357297
8	1.007265	-1.290853	0.378824
1	0.112304	-0.633211	-1.364811
6	4.792325	0.340864	-0.265158
6	4.074555	0.665315	0.885614
6	2.801187	0.137891	1.092790
6	2.256481	-0.718491	0.141141
6	2.966245	-1.059499	-1.006949
6	4.236581	-0.521719	-1.208762
1	5.781695	0.753920	-0.423346
1	4.504622	1.332152	1.624295
1	2.225393	0.378383	1.977742
1	2.532029	-1.747328	-1.723479
1	4.794431	-0.785439	-2.100068

(c) Vibrational frequencies.

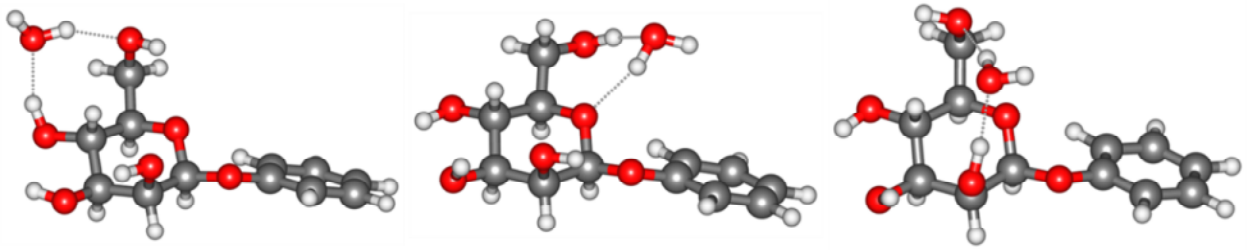
	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
ν1	24.0960	0.0645	28.5586	0.2286	20.0538	0.1654
ν2	42.6520	0.4448	43.3306	0.0591	30.7741	0.2355
ν3	49.9758	1.7419	58.4725	1.6052	46.7859	1.0959
ν4	86.1406	0.2047	82.6544	0.7130	81.5002	0.3732
ν5	109.4219	1.8831	92.6530	4.8824	105.1689	1.4483
ν6	121.7355	4.1949	124.1533	2.9812	119.0408	4.9136
ν7	158.7987	0.9498	148.8032	0.7042	140.8844	1.9860
ν8	180.2746	0.2612	210.4558	4.5733	181.3925	0.0813
ν9	217.5058	2.6800	229.3415	1.2294	198.6071	3.3504
ν10	229.5833	4.0428	235.4886	0.0706	228.7511	0.0543
ν11	242.5198	1.8412	256.1265	1.0219	241.0821	2.7303
ν12	264.9258	10.6265	262.8930	12.1774	262.6767	12.9874
ν13	272.3924	8.6722	268.9979	15.9422	286.7860	19.9403
ν14	304.8287	18.3491	276.6610	2.7782	326.3813	56.4120
ν15	327.6015	95.3915	314.1005	67.6503	356.4913	63.9287
ν16	360.2813	26.0063	358.5276	92.6874	377.9478	8.6011
ν17	387.2104	12.1776	373.1434	33.0668	388.2160	15.4606
ν18	401.5308	46.2681	405.6941	13.0905	404.3971	44.8160
ν19	412.2678	45.6646	409.0047	87.3558	415.9234	66.1777
ν20	419.2486	0.6034	420.6259	0.1685	423.9337	12.2995
ν21	432.1097	95.0562	429.6270	42.2733	424.4954	9.4401
ν22	461.2231	23.8720	485.1034	149.9522	456.5061	18.4086
ν23	491.6973	137.3281	492.0837	6.2750	472.3759	56.7938
ν24	513.8927	7.8238	512.5626	9.6745	499.8440	107.0604
ν25	520.5946	12.1942	522.8050	12.5696	533.3367	26.8671
ν26	558.7700	9.9208	574.0025	2.5587	563.5850	0.7005
ν27	615.4653	6.0949	602.4848	5.6603	615.5760	7.6239
ν28	616.2899	4.0675	634.2875	0.4984	616.9316	4.1203
ν29	642.4238	2.4166	682.7296	2.3824	632.7752	0.6582
ν30	697.5352	16.4731	699.5468	15.8837	701.0218	2.8652
ν31	703.6236	24.5095	704.7333	33.8982	708.3020	63.3619
ν32	763.4628	62.2650	765.8976	60.1827	775.4083	20.8113
ν33	796.4498	24.0692	803.8379	32.1940	799.4576	37.6691
ν34	828.1227	5.0355	832.8086	2.0045	840.1044	15.1486
ν35	839.6070	21.2890	853.6100	26.7505	843.4197	4.0314
ν36	879.6676	28.3457	887.4982	51.6806	876.9113	26.2796
ν37	892.9907	53.3130	893.5676	13.5039	891.2390	48.7078
ν38	900.9728	10.0977	906.6457	17.7618	926.1938	14.6880
ν39	943.2149	30.4153	912.2105	18.5958	943.1059	18.3262
ν40	971.7567	0.0863	961.6181	7.4559	980.6536	0.1255
ν41	989.9161	0.0467	974.0332	0.0796	999.1784	0.8883
ν42	1013.5325	7.0427	992.0867	0.1012	1016.2415	75.3012
ν43	1019.3685	81.0779	1014.6432	3.4316	1019.2275	22.6887
ν44	1037.9879	107.4559	1036.1764	233.2001	1037.6416	148.7020
ν45	1044.5899	69.7283	1038.5805	4.5033	1041.7845	29.9435
ν46	1055.0863	19.3718	1049.4991	18.0282	1051.7562	41.2544
ν47	1078.9049	130.4467	1063.6055	103.4675	1077.6299	224.1910
ν48	1079.7765	136.4722	1087.9194	208.0012	1080.9284	20.3452
ν49	1090.0005	119.2600	1093.1614	59.6860	1090.8886	116.5428
ν50	1102.2304	60.5588	1102.1734	62.3286	1092.8888	15.8075
ν51	1106.5878	86.6901	1105.9788	124.5824	1106.5743	140.8302
ν52	1126.4906	14.0634	1120.6452	32.3363	1125.9474	8.4161
ν53	1134.7658	23.9328	1134.6009	34.3898	1128.8026	11.6296
ν54	1165.2486	108.7296	1163.2711	107.1356	1167.0750	87.2366
ν55	1179.9297	1.5669	1180.1090	1.6607	1180.5628	0.2804
ν56	1197.4712	14.5011	1195.2595	12.0286	1182.9311	12.3966
ν57	1211.5600	62.7574	1212.5409	53.6007	1213.1285	69.4583
ν58	1221.3969	4.1821	1227.6835	15.2722	1222.7221	6.6356
ν59	1245.1658	11.3599	1243.2250	225.5285	1235.5272	173.4357
ν60	1249.8765	353.5159	1255.9042	134.4893	1243.2314	54.5034
ν61	1274.7727	29.0446	1272.1033	29.8911	1275.6993	50.1492
ν62	1298.7669	10.2059	1302.2130	5.6960	1298.3322	8.9538
ν63	1323.6114	4.7469	1327.9203	2.1848	1320.2733	1.9490
ν64	1328.7999	2.1174	1332.2914	4.3488	1322.9571	3.3478
ν65	1340.0942	23.0833	1337.3875	13.4795	1338.6314	8.3820
ν66	1353.7153	22.5319	1353.0985	6.1299	1343.3032	2.5380
ν67	1357.3333	79.9070	1357.1877	101.4086	1352.8339	108.6083
ν68	1372.2911	18.1741	1371.4489	7.0389	1368.9651	6.1506
ν69	1382.5334	17.7981	1381.5225	6.1072	1378.8941	21.2016
ν70	1397.2687	1.9746	1395.5495	12.1439	1395.6972	2.4941
ν71	1409.9415	18.1722	1403.0106	21.2716	1407.2755	12.9685
ν72	1415.6031	3.4990	1419.8814	10.8891	1414.6451	4.4441
ν73	1422.1094	8.9210	1426.3643	31.6341	1422.8036	4.2025
ν74	1436.4881	25.3566	1436.6586	12.5981	1436.8828	42.0318
ν75	1439.9691	38.9989	1442.0989	38.9869	1440.1165	27.3974

v76	1487.3180	0.6816	1487.3736	0.6959	1482.2084	1.9638
v77	1499.2632	2.4281	1496.2470	7.0839	1500.6382	2.7033
v78	1522.3990	103.1405	1522.2446	104.2828	1520.6909	69.2078
v79	1629.0739	28.9460	1629.3454	26.5723	1631.0074	8.9432
v80	1640.3269	54.9291	1640.0877	55.9980	1634.5341	34.7196
v81	2961.5723	20.9857	2961.1705	19.5003	2958.0897	21.7682
v82	2983.7647	8.0101	2974.6468	22.3492	2985.0606	4.8070
v83	3002.4790	12.3539	3004.0480	64.7776	2998.9526	23.1396
v84	3007.8516	46.1853	3007.1050	41.7978	3005.8031	45.6633
v85	3012.4560	52.4866	3036.7261	3.1991	3011.6534	46.8972
v86	3051.9660	34.6161	3053.3458	38.9519	3051.5072	34.8939
v87	3122.4189	9.6269	3116.2016	10.0090	3121.7267	9.8341
v88	3168.1445	1.1133	3168.0234	1.0609	3166.9437	1.1565
v99	3175.8708	7.8676	3175.7771	8.7948	3174.8113	5.3009
v90	3188.7829	16.7449	3188.9855	17.2315	3184.2713	16.8738
v91	3196.0896	9.0995	3196.2997	8.3148	3192.6734	11.5072
v92	3211.0667	1.7159	3214.2142	1.2995	3201.3416	1.7326
v93	3777.1537	60.2301	3780.4250	56.2684	3777.2805	61.9798
v94	3798.8304	60.6819	3808.7168	65.6573	3798.1973	60.3435
v95	3814.7220	63.8295	3810.5821	29.1345	3808.7133	67.2011
v96	3818.7645	48.3227	3815.9411	69.0709	3811.6074	57.4330

6. β-PhMan•$(D_2O)_1$

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

Conformer	B3LYP/6-311++G(d,p) energy / kJ mol^{-1}	MP2/6-311++G(d,p)//B3LYP/6-311++G(d,p) energy / kJ mol^{-1}
A	2.00	0.00
B	4.26	0.01
C	4.95	1.30



A B C

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

A			
6	-0.491083	0.694836	-0.249781
6	0.464881	1.870099	-0.025290
6	1.761548	1.596159	-0.796570
6	2.343038	0.241343	-0.399510
6	1.291545	-0.853952	-0.655888
8	0.102697	-0.555293	0.089407
8	0.720627	2.027587	1.356831
8	2.664772	2.652983	-0.494355
8	3.533720	0.042173	-1.148558
6	1.716336	-2.247648	-0.217365
8	2.070034	-2.302171	1.169548
1	1.467540	2.636240	1.425264
1	3.535992	2.368994	-0.800395
1	1.342194	-1.920161	1.676844
1	-0.014920	2.770446	-0.432965
1	1.549350	1.587355	-1.876129
1	2.566397	0.263115	0.670528
1	1.066605	-0.891212	-1.733930
1	4.145105	-0.480042	-0.598612
1	2.598611	-2.562267	-0.775213
1	0.902392	-2.950605	-0.423191
8	-1.624465	0.878704	0.534948
1	-0.767077	0.672886	-1.317439
6	-5.285568	-0.912897	-0.332929
6	-5.180782	0.157089	0.558078
6	-3.944872	0.732985	0.826032
6	-2.797252	0.235196	0.204020
6	-2.885734	-0.843555	-0.676453
6	-4.136096	-1.405174	-0.943202
1	-6.250603	-1.358845	-0.542499
1	-6.067422	0.549909	1.043051
1	-3.845004	1.568392	1.508321
1	-1.996483	-1.263669	-1.125435
1	-4.201596	-2.243899	-1.627493
8	4.722380	-1.601474	0.801420
1	3.906327	-1.912643	1.235978
1	5.408707	-1.560946	1.472544

B			
6	-0.124249	-0.772215	-0.296293
6	-1.212964	-1.824111	-0.052635
6	-2.549688	-1.311717	-0.590334
6	-2.854594	0.108209	-0.092860
6	-1.677381	1.043737	-0.390635
8	-0.490487	0.492339	0.223966
8	-1.399695	-2.091921	1.330516
8	-3.617039	-2.197261	-0.272340
8	-4.006731	0.620927	-0.748053
6	-1.882921	2.456499	0.149228
8	-0.841365	3.340187	-0.219333
1	-0.541430	-2.282043	1.726601
1	-3.495159	-2.474479	0.645805
1	-0.125821	3.244882	0.430163
1	-0.929015	-2.742310	-0.583312
1	-2.505748	-1.280550	-1.683971
1	-3.009189	0.078769	0.994150
1	-1.519108	1.104675	-1.476783
1	-4.694303	-0.053782	-0.687114
1	-2.812849	2.838316	-0.275165
1	-2.000321	2.410662	1.239652
8	1.027267	-1.210513	0.372612
1	0.071328	-0.685600	-1.376364
6	4.854504	0.062492	-0.687809
6	3.755552	0.796691	-1.123817
6	2.455896	0.411729	-0.786366
6	2.269441	-0.734796	-0.013941
6	3.363615	-1.477367	0.432102
6	4.651202	-1.074381	0.096062
1	5.858492	0.372070	-0.952258
1	3.899447	1.686318	-1.726426
1	1.614434	1.012883	-1.104109
1	3.189430	-2.363280	1.030859
1	5.498128	-1.655513	0.442725
8	0.916363	2.393700	1.835415
1	1.878085	2.364927	1.830844
1	0.626636	1.535759	1.486203

C			
6	0.198308	-0.612704	-0.451617
6	-0.871718	-1.696493	-0.271441
6	-2.143690	-1.252539	-1.017954
6	-2.572620	0.141725	-0.559002
6	-1.419742	1.140077	-0.702612
8	-0.266853	0.657472	-0.005396
8	-1.178895	-2.008207	1.071985
8	-3.202999	-2.178912	-0.814821
8	-3.676097	0.628978	-1.316244
6	-1.738157	2.516377	-0.130032
8	-2.146935	2.459470	1.244739
1	-1.201102	-1.208391	1.638785
1	-3.111369	-2.494445	0.097396
1	-3.108181	2.437217	1.284762
1	-0.498040	-2.620271	-0.722763
1	-1.957862	-1.227598	-2.097680
1	-2.848740	0.077916	0.500453
1	-1.190147	1.265251	-1.773340
1	-4.318782	-0.090144	-1.368204
1	-2.509425	2.990287	-0.740854
1	-0.834311	3.127393	-0.161241
8	1.318359	-0.956557	0.301116
1	0.461086	-0.544058	-1.520820
6	5.114336	0.600315	-0.434023
6	4.011405	1.218357	-1.015072
6	2.719298	0.738951	-0.790481
6	2.540510	-0.384490	0.017146
6	3.641026	-1.009554	0.608542
6	4.919999	-0.514663	0.383566
1	6.112489	0.983421	-0.609930
1	4.147048	2.092028	-1.642958
1	1.869496	1.255394	-1.214298
1	3.472301	-1.878853	1.232555
1	5.769485	-1.005890	0.844733
8	-1.413492	0.178581	2.851826
1	-1.482264	1.018098	2.361383
1	-0.630118	0.263908	3.404250

(c) Vibrational frequencies.

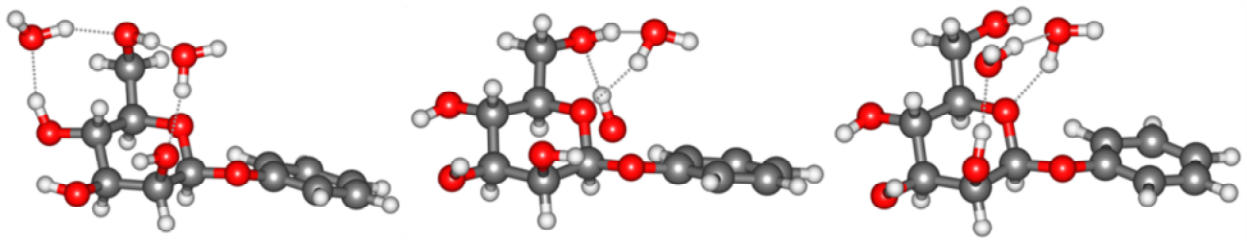
	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
ν1	27.1941	0.1546	25.1831	0.8167	28.8077	0.2507
ν2	41.9102	0.6814	38.8186	1.7485	39.7229	4.2637
ν3	44.2472	0.8193	49.5707	1.5787	47.6882	0.3280
ν4	63.6657	0.3491	56.2056	0.9043	62.0200	1.7380
ν5	83.8883	2.2489	79.8573	3.2530	85.6992	6.8456
ν6	91.3726	2.6247	95.9642	7.2195	106.4193	6.8111
ν7	123.3869	61.9673	117.2192	4.6164	117.4563	2.0647
ν8	132.1578	18.4490	131.3942	1.4165	149.7284	14.6406
ν9	153.3016	1.6637	160.2325	4.9043	160.6210	2.6015
ν10	178.2284	23.5067	170.1798	36.5695	173.2529	18.2507
ν11	208.8405	11.6521	191.2126	3.7985	188.8020	29.1773
ν12	212.9907	10.0563	200.5347	15.6408	219.9033	1.8236
ν13	228.7727	1.5342	218.2182	1.8037	231.7473	6.0856
ν14	248.6127	7.4234	232.2399	1.6685	236.8091	0.6826
ν15	260.2878	1.6395	250.1205	5.3958	255.0252	49.8216
ν16	263.9582	7.2155	263.1870	23.8951	262.5845	26.1547
ν17	275.9438	13.4808	269.7431	9.0786	264.7510	66.0122
ν18	279.1695	7.6922	276.7719	35.4224	272.0591	35.7385
ν19	331.7733	7.3007	300.8525	9.9262	285.7756	3.0908
ν20	346.9521	31.4510	331.7578	82.9059	338.5819	1.1229
ν21	401.5617	9.9430	354.9504	22.4505	373.5413	77.6233
ν22	409.1683	45.1901	371.3084	47.9481	394.3047	19.6077
ν23	420.8193	1.0471	396.8204	47.5546	417.8268	11.6580
ν24	428.2792	75.0503	401.6968	11.6479	420.9836	0.1159
ν25	438.5793	27.7432	418.4912	3.1535	435.5654	35.9248
ν26	455.9167	146.9257	422.5752	0.1602	483.5737	37.1761
ν27	478.6079	68.7388	460.7302	25.7506	493.0136	13.3644
ν28	496.7741	42.0086	489.5638	124.9291	513.4759	3.7184
ν29	515.2245	10.5308	510.8617	21.7874	523.5060	11.7838
ν30	524.1412	19.9940	521.9866	3.0912	546.0762	97.5058
ν31	574.1184	3.0663	557.7445	9.5013	572.7982	4.3778
ν32	604.1083	11.1368	609.2823	5.9773	607.3484	2.1385
ν33	635.3293	3.1595	616.6313	7.1223	636.1824	0.5639
ν34	677.7687	4.9585	638.0576	14.6274	674.0851	0.4485
ν35	698.6351	16.5627	658.8792	154.6823	699.4086	21.8547
ν36	702.1819	15.8078	701.5468	8.6654	720.8520	15.2701
ν37	733.3977	115.4370	705.1595	25.7589	764.4492	70.0942
ν38	764.2284	58.6591	766.7576	61.3617	768.2705	126.3714
ν39	797.8560	32.4980	796.2055	29.4369	806.8934	19.6712
ν40	831.5222	5.4459	836.9526	18.6825	832.2440	4.5330
ν41	840.9898	39.9680	841.0286	8.6300	842.4846	12.3329
ν42	885.6185	52.5898	882.8028	35.8943	878.4613	13.7026
ν43	895.2429	0.5767	890.2708	42.6268	891.2461	45.2394
ν44	904.3373	23.0795	911.7784	9.9922	903.3589	4.0906
ν45	913.9685	23.5790	943.0990	35.6309	906.5884	48.5224
ν46	962.8461	27.6349	979.5832	0.0488	948.0639	42.0302
ν47	972.4845	0.3474	996.2507	0.1020	972.9389	0.1032
ν48	989.0731	0.1703	1013.6666	30.8621	989.1857	0.1481
ν49	1013.8550	5.4358	1016.1073	67.5577	1013.9493	8.7079
ν50	1029.6061	273.5793	1037.0243	97.2181	1021.8362	227.6158
ν51	1044.1215	22.2545	1047.2038	111.7880	1039.4348	5.0587
ν52	1057.7387	37.1390	1054.7688	24.9887	1050.6386	42.4333
ν53	1064.6879	102.6657	1075.2749	98.4025	1079.3585	204.0911
ν54	1082.6590	176.7095	1085.9183	226.2288	1084.6327	151.2786
ν55	1095.8025	87.9734	1089.1925	44.6124	1090.0850	78.7178
ν56	1103.7690	23.8539	1103.0759	25.8172	1101.0085	30.5951
ν57	1122.6745	19.2507	1105.2255	67.2913	1103.3869	42.2652
ν58	1125.2600	30.2211	1122.7911	18.3865	1120.6477	35.6605
ν59	1141.0718	69.6699	1137.1798	20.3340	1149.9321	21.0440
ν60	1156.4765	38.5204	1164.2897	94.3477	1168.2721	62.5832
ν61	1178.9634	3.3458	1180.7358	1.9948	1179.4161	1.9301
ν62	1190.8059	25.5833	1192.6757	57.2699	1195.5248	18.3855
ν63	1194.8319	16.0431	1197.3308	15.5460	1201.9410	19.3116
ν64	1219.8539	79.8309	1209.9537	61.6868	1220.2393	74.8662
ν65	1233.7346	36.9152	1223.4202	10.9635	1247.8211	49.6295
ν66	1250.6862	192.1648	1246.2316	283.6149	1256.1555	311.0513
ν67	1262.0839	149.1187	1268.3974	57.4522	1270.3151	46.5478
ν68	1275.5951	52.3430	1278.5481	23.0907	1286.4766	6.6012
ν69	1294.8496	1.2233	1297.4071	9.8885	1300.7508	20.7919
ν70	1327.5814	4.3121	1321.5948	3.3495	1315.6426	5.6452
ν71	1334.7931	15.3610	1327.7269	1.4236	1330.8313	3.7295
ν72	1342.6750	28.8399	1347.0765	28.7657	1340.5805	25.1804
ν73	1354.7156	10.8459	1353.3913	40.5561	1346.2449	21.1571
ν74	1366.3720	11.9222	1355.5685	49.1840	1353.9680	7.6246
ν75	1392.5507	17.9037	1375.2262	17.4623	1384.7515	16.1761

v76	1394.0846	7.0965	1394.5093	9.8530	1394.2474	11.3140
v77	1403.2146	14.6079	1403.8080	18.5437	1399.8524	40.1665
v78	1411.3719	4.5133	1414.8004	1.9990	1405.5538	20.2300
v79	1419.0099	52.4096	1418.0193	8.7025	1420.8821	36.8021
v80	1426.5552	33.3609	1432.4251	9.9082	1431.8859	22.1885
v81	1446.2290	36.8647	1440.0241	44.4302	1440.2649	17.2675
v82	1456.9073	24.9234	1460.6528	22.2212	1449.7490	54.4397
v83	1486.7711	0.5537	1487.3614	1.0887	1485.8094	8.9657
v84	1501.7081	8.0005	1494.9044	3.9289	1486.7134	1.2126
v85	1522.6985	105.2427	1521.9962	98.0817	1522.3661	105.0109
v86	1627.0824	24.6164	1627.9534	26.4239	1627.5758	24.8057
v87	1640.7914	65.9257	1639.5738	49.0959	1640.5667	62.1881
v88	2615.1091	162.6930	2680.9663	97.2732	2630.5333	144.9909
v89	2845.8192	89.7756	2838.9215	68.9042	2829.6082	66.0600
v90	2948.6660	18.2061	2972.5160	16.0001	2946.0268	28.0049
v91	2966.5629	15.1909	2993.3088	1.9688	2965.3966	29.2072
v92	2981.8761	34.8759	3003.1825	8.8081	3019.6461	8.9875
v93	3003.8130	65.0041	3009.7388	40.0562	3040.3379	32.0935
v94	3037.5412	40.2567	3015.3246	54.1098	3060.2919	38.4568
v95	3066.6003	15.1127	3052.7014	33.3739	3061.3878	31.7432
v96	3117.6836	10.7055	3103.1707	14.3230	3111.8754	14.2731
v97	3165.1636	1.1645	3169.6045	0.8278	3165.5546	1.1760
v98	3173.3159	11.9230	3177.5691	7.4053	3173.4907	11.5158
v99	3188.6400	20.9754	3189.8660	14.5864	3188.7563	19.9457
v100	3197.2739	5.7105	3196.9013	7.0805	3196.6646	6.1183
v101	3211.9881	3.4858	3207.1186	0.3196	3214.6304	3.7106
v102	3625.9263	506.7730	3672.6187	315.8448	3501.8970	533.6398
v103	3787.4161	103.2186	3778.8541	60.2065	3730.6407	64.1110
v104	3789.3321	29.0854	3799.0316	59.2089	3791.1041	65.8017
v105	3795.1474	59.6204	3820.4831	62.5696	3843.9665	59.5281

7. β-PhMan•$(D_2O)_2$

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

Conformer	B3LYP/6-311++G(d,p) energy / kJ mol^{-1}	MP2/6-311++G(d,p)//B3LYP/6-311++G(d,p) energy / kJ mol^{-1}
A	0.00	0.00
B	13.30	10.82
C	15.41	11.92



A B C

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

A			
6	-0.594053	0.736856	-0.366145
6	0.363728	1.887106	-0.059011
6	1.626665	1.695019	-0.899175
6	2.242797	0.321634	-0.642345
6	1.195933	-0.789045	-0.862831
8	0.007712	-0.516521	-0.097971
8	0.676584	1.881384	1.333258
8	2.531852	2.733894	-0.542013
8	3.361397	0.190393	-1.506045
6	1.669116	-2.174176	-0.426634
8	2.282886	-2.202920	0.858456
1	1.431166	2.475366	1.447071
1	3.390644	2.493780	-0.914273
1	1.739526	-1.732108	1.526578
1	-0.123648	2.831897	-0.326117
1	1.366498	1.775650	-1.964525
1	2.570004	0.287205	0.400023
1	0.944721	-0.833330	-1.934293
1	4.029844	-0.360546	-1.054021
1	0.809537	-2.853244	-0.457742
1	2.416773	-2.537654	-1.134244
8	-1.725516	0.870247	0.439350
1	-0.877736	0.789685	-1.430730
6	-5.372094	-0.916522	-0.500997
6	-5.276860	0.113407	0.436780
6	-4.046106	0.689828	0.728057
6	-2.895476	0.231728	0.082209
6	-2.973956	-0.806793	-0.845962
6	-4.219033	-1.368694	-1.135295
1	-6.332842	-1.362857	-0.728535
1	-6.166548	0.474946	0.940092
1	-3.955036	1.496330	1.445631
1	-2.080790	-1.197356	-1.313375
1	-4.277288	-2.176472	-1.856378
8	1.070804	-0.591748	2.804193
1	0.267477	-0.881357	3.247904
1	0.819665	0.223229	2.330419
8	4.811457	-1.530171	0.129011
1	4.029599	-1.856586	0.624485
1	5.537049	-1.455140	0.754191

B			
6	-0.194753	-0.883204	-0.377913
6	-1.322646	-1.923866	-0.353793
6	-2.655758	-1.259376	-0.702949
6	-2.885993	0.013372	0.123511
6	-1.682257	0.949663	-0.020014
8	-0.504096	0.243267	0.427374
8	-1.482557	-2.509600	0.931847
8	-3.745753	-2.161530	-0.551570
8	-4.044617	0.697053	-0.335595
6	-1.817476	2.225441	0.803970
8	-0.738668	3.133689	0.588766
1	-0.616439	-2.791168	1.249071
1	-3.594442	-2.657097	0.264794
1	-0.013924	2.882878	1.193189
1	-1.089914	-2.697668	-1.097026
1	-2.648109	-0.974621	-1.760097
1	-2.993860	-0.261817	1.181150
1	-1.550737	1.223782	-1.074890
1	-4.750033	0.042345	-0.411226
1	-2.738404	2.725649	0.503338
1	-1.894343	1.972108	1.867292
8	0.937364	-1.507370	0.159228
1	-0.010865	-0.556422	-1.411298
6	4.831686	-0.123954	-0.406984
6	4.565604	-1.321705	0.258833
6	3.255534	-1.753537	0.431197
6	2.202119	-0.982324	-0.063580
6	2.447051	0.220451	-0.725154
6	3.771290	0.634740	-0.893619
1	5.853111	0.211297	-0.542807
1	5.380072	-1.924852	0.643789
1	3.032871	-2.683201	0.941147
1	1.650950	0.849893	-1.103186
1	3.959364	1.568781	-1.410843
8	0.443205	2.687824	-1.909036
1	0.029328	3.014333	-1.085020
1	0.492801	3.443623	-2.500723
8	1.087559	1.794368	2.225030
1	0.757823	1.015752	1.746800
1	2.038844	1.800585	2.077178

C			
6	0.015043	-0.829724	-0.469543
6	-1.111944	-1.829914	-0.201718
6	-2.373012	-1.338473	-0.937292
6	-2.706077	0.115556	-0.580946
6	-1.491154	1.028315	-0.781371
8	-0.374126	0.478916	-0.046667
8	-1.386962	-2.052651	1.166620
8	-3.483477	-2.178721	-0.650305
8	-3.763963	0.604302	-1.396185
6	-1.748134	2.444705	-0.269859
8	-0.621742	3.297009	-0.406001
1	-1.352339	-1.227803	1.691112
1	-3.394229	-2.436586	0.279413
1	-0.074802	3.192790	0.383031
1	-0.816263	-2.798945	-0.614072
1	-2.215750	-1.397925	-2.020103
1	-2.994353	0.159506	0.478577
1	-1.224489	1.070040	-1.846442
1	-4.473272	-0.049549	-1.359860
1	-2.559628	2.867364	-0.863849
1	-2.081226	2.395795	0.773294
8	1.148892	-1.198933	0.250627
1	0.233598	-0.802386	-1.548285
6	4.975354	0.138726	-0.727037
6	3.875934	0.806662	-1.256938
6	2.574180	0.399307	-0.954378
6	2.385300	-0.703112	-0.119622
6	3.482017	-1.378480	0.420948
6	4.770405	-0.954708	0.116952
1	5.980619	0.465415	-0.965092
1	4.020238	1.662647	-1.906476
1	1.732446	0.953372	-1.347493
1	3.303183	-2.230699	1.065366
1	5.618035	-1.485088	0.536070
8	0.565468	1.923816	2.064546
1	1.490622	1.925789	2.330737
1	0.498020	1.320793	1.298583
8	-1.484918	0.156910	2.946264
1	-0.781948	0.829833	2.889981
1	-1.589281	-0.052687	3.879132

(c) Vibrational frequencies.

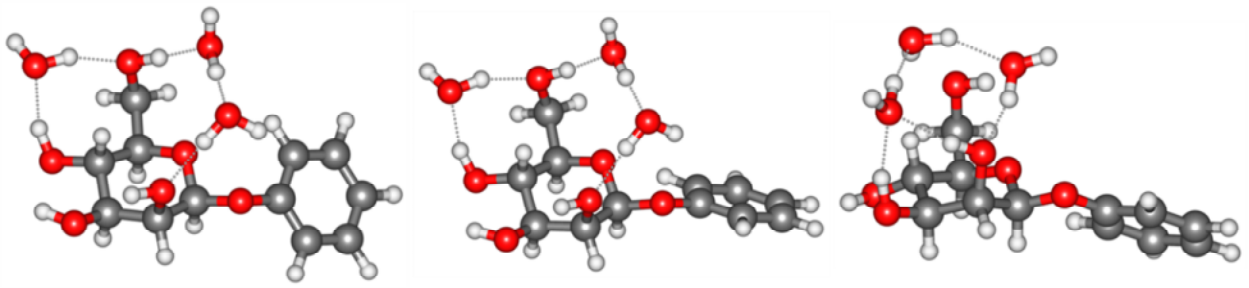
	A		B		C	
	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}	Frequency / cm^{-1}	Intensity / km mol^{-1}
ν1	25.8879	0.0564	28.9101	0.1217	22.3015	0.9589
ν2	39.4920	1.3099	44.1936	1.5433	37.9045	2.4463
ν3	43.9797	0.1864	50.0349	2.5590	46.4357	0.3181
ν4	53.8864	4.8545	58.8397	0.3254	51.9785	0.2093
ν5	67.1667	0.1459	62.3685	0.1822	54.4093	0.2546
ν6	89.5318	1.8038	79.6828	3.4702	83.9406	5.8793
ν7	107.4623	4.4883	86.2592	1.9545	95.1231	0.0888
ν8	121.4725	11.3453	101.5209	4.3241	113.5726	3.5153
ν9	143.9880	26.2257	121.3401	3.0866	130.2891	1.5443
ν10	153.5480	0.7634	125.3065	71.0365	148.8476	14.4992
ν11	160.5867	36.8721	133.2892	2.0778	160.8488	16.3807
ν12	180.0387	29.1007	149.6807	0.4366	162.3108	13.2679
ν13	183.2452	36.5238	176.2437	6.1369	178.0865	3.0380
ν14	198.5451	14.6511	199.7354	42.9037	187.4373	5.9651
ν15	217.9346	11.6274	207.7369	5.8506	203.3902	19.2109
ν16	229.0200	3.8623	218.1822	2.6682	220.0986	6.2065
ν17	242.8533	7.4581	232.4162	10.2526	228.6542	13.3197
ν18	249.1711	4.2033	236.9371	5.1576	249.0264	7.9141
ν19	268.2516	11.5395	246.5679	11.7652	258.0630	23.2988
ν20	274.1322	43.0067	264.9652	18.8347	268.2105	2.8605
ν21	278.2645	6.5048	276.1861	9.1410	275.8632	12.2475
ν22	287.9082	2.8570	298.6473	84.7125	282.3992	64.3417
ν23	298.8878	21.4999	301.5249	8.7655	305.6944	3.3564
ν24	335.7818	2.5457	308.8028	13.1457	337.4850	43.1007
ν25	368.5099	35.5135	335.2906	83.6464	356.7737	14.8316
ν26	408.2584	4.1380	365.5793	13.8043	394.9498	4.8983
ν27	420.7467	6.5119	390.4399	61.5865	405.1282	51.1853
ν28	421.4068	16.3555	401.0716	40.2968	407.8296	27.6239
ν29	455.0244	118.9633	404.5095	17.0574	422.7966	2.2757
ν30	467.7253	126.1511	422.0065	0.0948	423.3724	4.9668
ν31	485.1303	11.3627	425.1752	1.5705	465.6730	12.5353
ν32	498.5056	23.8035	465.2935	19.4146	482.5355	175.4886
ν33	515.8187	2.5689	496.4282	125.8755	508.5495	9.4479
ν34	523.7600	24.5254	514.7471	32.0256	518.1700	41.7241
ν35	530.8620	48.3163	518.8700	15.2693	523.1874	20.8296
ν36	575.2091	3.1347	525.7862	28.5738	559.1606	6.7953
ν37	604.9998	3.4851	560.1799	10.0553	589.7854	39.7220
ν38	635.8816	1.0589	613.1298	1.3965	614.3696	7.3871
ν39	674.5052	4.0669	619.2919	9.7099	620.4870	13.7618
ν40	699.5941	19.4406	638.9275	1.7347	644.4809	4.6415
ν41	709.2126	27.2024	701.4649	16.0194	703.4219	18.3320
ν42	763.9481	61.9668	703.4674	25.8374	714.7494	132.2344
ν43	765.9613	75.5700	767.1301	94.5487	720.2993	21.4152
ν44	799.3288	28.8825	776.3530	105.7424	766.5562	66.0621
ν45	828.6403	153.9260	796.4086	32.5454	794.3047	19.1369
ν46	832.9230	9.8491	838.8370	25.3811	833.7089	19.2177
ν47	840.9121	30.7651	848.3302	2.2126	841.2439	2.0450
ν48	887.6463	37.9063	881.9879	36.9214	880.9574	22.1798
ν49	894.8755	6.2279	891.3921	49.9351	888.2388	72.9088
ν50	906.1064	30.3164	923.0746	5.1278	911.0360	11.4661
ν51	916.3602	9.6110	944.3484	35.4436	934.2368	48.1230
ν52	968.3579	30.7941	982.3127	0.0628	979.9160	0.0573
ν53	973.1739	1.0464	1003.7962	0.9525	994.3613	0.1693
ν54	990.4430	0.1268	1011.6503	12.8770	1010.0835	155.3223
ν55	1014.2288	4.2654	1015.7130	81.3654	1014.3424	14.6150
ν56	1037.7239	206.7631	1035.6454	103.7289	1038.2602	65.9958
ν57	1046.9007	105.6352	1045.6871	48.9635	1045.4609	102.1829
ν58	1068.1709	65.7632	1057.9874	26.4940	1051.4005	19.7861
ν59	1071.5395	79.3460	1074.0463	203.3436	1069.1726	48.9577
ν60	1087.5217	142.0228	1083.8907	9.2098	1080.6192	270.9345
ν61	1093.4925	75.4048	1090.4237	201.7790	1093.0506	43.9406
ν62	1103.4410	11.5503	1106.3097	36.7407	1096.6253	57.9922
ν63	1124.3578	19.8525	1108.2719	63.1065	1102.9663	3.2041
ν64	1129.8393	70.6468	1127.1640	18.2340	1130.5692	7.1892
ν65	1133.1114	38.5014	1140.4945	17.8104	1149.1356	14.2555
ν66	1156.6098	23.4555	1166.6472	83.3805	1168.9750	66.5672
ν67	1179.2520	3.4389	1179.1163	1.8578	1178.8395	56.1683
ν68	1195.0254	13.9396	1193.9371	66.8843	1180.6262	24.1427
ν69	1196.6148	26.6942	1196.3316	25.5636	1197.2959	17.4135
ν70	1206.7932	50.0176	1204.6015	17.9152	1208.0579	24.6468
ν71	1224.9345	58.6145	1215.2345	62.4769	1219.7844	34.1388
ν72	1246.4183	166.5560	1229.5367	19.1882	1249.9535	277.9128
ν73	1256.5683	173.7852	1244.6653	302.5059	1262.9959	123.9520
ν74	1264.2443	19.8477	1273.1402	60.8357	1274.0093	9.4701
ν75	1280.1456	54.7791	1281.1263	20.8248	1281.6655	20.2205

v76	1303.7133	0.8506	1304.3482	5.5687	1296.1715	17.0888
v77	1327.9809	5.0881	1327.9969	4.7036	1310.6219	11.4328
v78	1334.3078	14.8387	1329.0502	3.1076	1326.8507	5.1335
v79	1341.7843	32.2194	1351.9893	36.0244	1336.0376	17.7638
v80	1354.2493	8.5308	1357.4798	41.2949	1350.2610	23.0205
v81	1378.2983	6.2993	1362.0109	33.4965	1355.0530	2.7726
v82	1387.4275	15.2135	1377.2261	22.2895	1393.9083	10.3783
v83	1391.4425	13.6358	1397.4816	12.5494	1400.2970	45.8718
v84	1399.6094	12.1085	1405.3596	11.1132	1413.4263	39.4654
v85	1410.9816	4.2294	1417.9822	3.5348	1414.8786	18.8890
v86	1422.7835	51.1486	1422.8938	4.0546	1422.5701	4.3359
v87	1445.4592	41.8540	1439.2721	17.6045	1431.8495	15.3843
v88	1449.1478	51.9743	1442.1245	39.1574	1435.2521	37.7312
v89	1469.7346	21.7425	1478.2945	21.6057	1446.9261	49.0402
v90	1486.9588	0.7231	1486.7733	2.8718	1486.5259	1.2990
v91	1498.3998	6.3729	1497.8155	7.1013	1497.4160	4.1001
v92	1522.4955	102.8504	1522.9217	86.9123	1521.9241	97.1185
v93	1627.4304	25.3005	1628.2582	33.8181	1626.4893	25.0459
v94	1640.4128	63.3993	1638.2290	36.8591	1639.6864	52.0632
v95	2534.3395	275.0852	2572.5171	220.9819	2586.9689	158.9038
v96	2623.7130	177.7013	2674.2635	100.0577	2631.5834	205.7359
v97	2828.4438	66.0540	2832.3110	64.7144	2825.4117	73.3071
v98	2840.7640	79.1692	2835.1642	62.2341	2836.0959	72.4168
v99	2949.2420	22.5715	2995.3133	6.1565	2972.5294	21.5077
v100	2971.9940	19.6897	3003.5681	9.5130	2993.8730	1.0930
v101	2990.8613	36.7905	3010.5564	40.7969	3006.0432	19.7638
v102	3026.7802	48.0364	3017.6411	9.8455	3029.5818	27.6844
v103	3032.7438	41.7904	3034.9256	28.8346	3039.8614	34.1710
v104	3067.9215	16.8690	3055.1846	32.0495	3062.1784	38.6591
v105	3096.2645	20.0284	3115.4160	11.7338	3108.3467	12.7415
v106	3166.1085	1.1231	3168.2194	0.3517	3168.3280	0.7502
v107	3173.9703	10.7138	3177.1158	13.0456	3176.5620	9.3309
v108	3188.6905	18.9740	3187.7741	21.9712	3190.1406	16.0979
v109	3196.0220	7.1163	3194.6393	1.3533	3197.5105	5.5561
v110	3214.3274	2.5236	3197.2597	20.9006	3209.8544	0.5466
v111	3488.2312	530.9600	3573.6173	450.4043	3555.4037	469.1819
v112	3565.3604	630.2536	3775.9128	61.8679	3739.8670	57.9228
v113	3776.8962	90.7013	3796.7535	61.0078	3775.4979	131.6142
v114	3786.6872	60.0903	3816.7584	66.1165	3798.4925	61.7213

8. β-PhMan•$(D_2O)_3$

(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	2.70	0.00
B	0.00	2.57
C	4.22	4.94



A B C

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

A			
6	5.042762	-0.693192	-0.807716
6	5.168531	0.687663	-0.986592
6	4.103139	1.530797	-0.655299
6	2.910911	1.005701	-0.147826
6	2.796710	-0.377768	0.015989
6	3.854818	-1.230785	-0.304521
8	1.651141	-0.939715	0.580468
6	0.518336	-1.037525	-0.241892
6	-0.464264	-2.027639	0.394160
6	-1.765520	-2.023968	-0.415366
6	-2.298084	-0.603497	-0.610710
6	-1.204504	0.268871	-1.253962
8	-0.049055	0.250680	-0.399184
6	-1.597865	1.730652	-1.466035
8	-2.178512	2.355332	-0.328812
8	-3.474696	-0.707971	-1.401837
8	-2.702432	-2.824242	0.301031
8	-0.723549	-1.660638	1.747361
8	-4.737441	1.454277	-0.221760
8	-0.368635	2.815739	1.654807
8	0.385274	0.581641	3.051395
1	-0.937004	-0.147470	-2.241638
1	-2.536760	-0.178984	0.371502
1	-1.576460	-2.469131	-1.405304
1	-0.012292	-3.029448	0.370168
1	0.811206	-1.422892	-1.235589
1	-1.561850	-2.091725	1.995311
1	-3.578456	-2.621603	-0.073951
1	-4.093753	0.002119	-1.114107
1	-0.709383	2.284914	-1.796337
1	-2.345577	1.775225	-2.264025
1	-1.502309	2.496385	0.384719
1	6.093270	1.104692	-1.376431
1	4.198866	2.605729	-0.785715
1	2.078578	1.648398	0.118350
1	3.741461	-2.299677	-0.146724
1	5.869172	-1.354291	-1.055817
1	-5.391068	2.067182	-0.587758
1	-3.887125	1.953662	-0.138695
1	1.331930	0.445188	2.889744
1	-0.033062	-0.199104	2.625026
1	-0.109742	1.997720	2.156226
1	-0.656208	3.456430	2.321912

B			
6	-0.556630	0.903980	-0.320883
6	0.349917	1.990119	0.270664
6	1.661709	2.021808	-0.518980
6	2.289039	0.630319	-0.614119
6	1.267248	-0.356416	-1.208838
8	0.086809	-0.356907	-0.383950
8	0.605393	1.722205	1.647323
8	2.531008	2.927091	0.155527
8	3.463376	0.761641	-1.404006
6	1.766929	-1.799039	-1.310778
8	2.419574	-2.286372	-0.147928
1	1.407758	2.223552	1.881848
1	3.424017	2.764534	-0.198264
1	1.777427	-2.454400	0.592011
1	-0.165384	2.956775	0.177963
1	1.461214	2.388463	-1.538508
1	2.543741	0.287220	0.395378
1	0.996553	-0.028733	-2.228763
1	4.133673	0.125058	-1.062259
1	0.917436	-2.443490	-1.573739
1	2.498809	-1.849290	-2.123101
8	-1.697721	0.791373	0.484572
1	-0.850448	1.214029	-1.339876
6	-5.329423	-0.659113	-0.984132
6	-4.146461	-1.021391	-1.630910
6	-2.907074	-0.561384	-1.171874
6	-2.866505	0.283537	-0.059122
6	-4.044740	0.653051	0.599152
6	-5.271181	0.176781	0.136586
1	-6.285974	-1.027101	-1.344483
1	-4.177757	-1.680882	-2.494507
1	-1.989521	-0.884757	-1.649222
1	-3.982332	1.314440	1.458561
1	-6.184314	0.466890	0.649871
8	0.766530	-2.786513	1.939858
1	0.345045	-1.974259	2.326844
1	1.167118	-3.261538	2.682554
8	-0.417762	-0.554792	2.994830
1	0.001242	0.235089	2.589218
1	-1.311451	-0.543830	2.616949
8	4.905226	-1.200994	-0.098659
1	5.601292	-1.775615	-0.448247
1	4.095416	-1.759518	0.008643

C			
6	0.668120	-0.102715	-0.805219
6	-0.488099	-0.982809	-1.296096
6	-1.551208	-0.039793	-1.887235
6	-1.984333	1.020721	-0.870700
6	-0.791598	1.726993	-0.207171
8	0.222332	0.794527	0.199855
8	-0.942162	-1.754993	-0.187122
8	-2.685246	-0.707186	-2.427983
8	-2.765672	2.034723	-1.499030
6	-1.198734	2.466136	1.069289
8	-1.768118	1.597291	2.043593
1	-1.861579	-2.070649	-0.316831
1	-3.195643	-1.125795	-1.701826
1	-1.135681	0.876374	2.245538
1	-0.117797	-1.651770	-2.085349
1	-1.091529	0.469020	-2.744818
1	-2.572744	0.532047	-0.085384
1	-0.369550	2.449255	-0.925815
1	-3.426066	1.585507	-2.053879
1	-1.960354	3.211489	0.827038
1	-0.318407	2.979593	1.480666
8	1.654270	-0.925447	-0.253950
1	1.082982	0.466754	-1.655055
6	5.629816	0.289254	0.151035
6	4.643874	1.259723	-0.033286
6	3.297261	0.901123	-0.165686
6	2.946333	-0.452049	-0.126303
6	3.926163	-1.433975	0.062776
6	5.261717	-1.060278	0.203099
1	6.671508	0.578728	0.257623
1	4.914577	2.312210	-0.063444
1	2.536688	1.666861	-0.264348
1	3.623807	-2.476809	0.088901
1	6.018249	-1.827515	0.346898
8	-3.605143	-0.672691	2.237943
1	-3.399681	0.278905	2.140792
1	-2.763154	-1.028199	2.594348
8	-3.727551	-1.984432	-0.113760
1	-4.378622	-2.701743	-0.096673
1	-3.797832	-1.496083	0.758492
8	-0.857373	-1.103793	2.513983
1	-0.700180	-1.326483	1.564336
1	-0.117552	-1.479669	3.013558

(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}
ν1	18.4588	0.3000	23.0575	0.1548	26.3341	0.0870
ν2	32.2233	0.3784	32.0087	0.2621	44.3151	0.4176
ν3	42.2270	0.8983	38.8347	0.3196	49.0750	0.6269
ν4	51.4619	0.7572	51.5659	0.8621	64.3191	2.1278
ν5	53.2540	0.9822	56.6573	0.9607	75.2603	1.8233
ν6	59.8310	1.7784	65.2416	1.7045	87.1670	0.7505
ν7	71.3070	0.8592	68.3675	0.8984	96.2015	1.9644
ν8	83.6566	7.0844	83.9578	5.6917	101.8684	1.4469
ν9	104.8307	0.5762	103.0674	0.9863	116.6381	2.0452
ν10	124.5658	7.1448	123.7059	8.2849	137.9146	10.5005
ν11	141.0789	5.9589	143.2530	4.3474	148.0680	4.7932
ν12	147.3980	3.3600	157.4593	0.8015	176.5414	10.8612
ν13	177.5879	21.4196	178.6506	23.9197	183.6136	19.1237
ν14	182.2949	19.3561	183.4851	11.4190	185.3244	9.0439
ν15	196.7981	20.8739	196.7353	53.2113	195.4303	2.5146
ν16	204.9594	40.9985	206.9143	23.4626	210.6202	20.1925
ν17	213.2149	34.5919	219.4605	33.6947	224.3589	13.4407
ν18	235.9378	10.7586	229.3431	11.0065	231.1058	6.6562
ν19	248.6906	43.8933	249.3965	9.8477	238.5051	20.5190
ν20	256.1097	27.9958	251.7121	37.2994	249.4762	4.4453
ν21	262.9275	21.0947	263.1326	40.9590	262.8520	3.8550
ν22	266.6944	7.8665	269.1847	10.2829	270.3258	24.4930
ν23	277.5151	24.9711	271.7278	12.4718	274.7139	12.8475
ν24	294.1375	0.6644	288.8891	13.4512	280.4376	11.5828
ν25	300.1625	34.0952	291.4649	29.0170	292.2519	15.2352
ν26	318.5733	4.0780	298.0445	0.7181	310.0193	2.4347
ν27	325.5030	21.3606	332.4573	26.4711	336.3345	17.7250
ν28	341.7935	38.4293	337.4782	11.1438	347.5592	14.5292
ν29	364.1196	2.4192	348.8070	27.9344	369.4567	36.9763
ν30	374.0192	9.4895	385.1757	7.6805	389.7258	44.2659
ν31	409.5145	1.1499	410.4873	0.9408	409.6460	30.8437
ν32	415.4545	22.6852	422.6228	19.3496	422.9161	0.8073
ν33	427.3643	0.3113	423.7394	0.7389	423.2736	37.4669
ν34	447.2550	61.9517	455.9270	86.4965	429.5855	13.5591
ν35	469.2243	46.1173	477.6531	105.7300	486.4087	1.1166
ν36	482.4250	118.2381	489.6413	23.8013	509.6087	43.7682
ν37	516.5097	55.4761	514.8524	37.9381	519.3186	18.7157
ν38	525.5833	2.8913	522.0169	36.3841	541.1502	78.5432
ν39	553.9044	48.8526	539.6429	30.4766	573.3674	0.7202
ν40	578.5893	38.4785	572.1794	4.2140	582.1703	120.4537
ν41	579.5768	15.9276	586.9583	47.3878	596.7451	4.4022
ν42	606.2888	2.9691	605.9222	4.5133	632.4853	4.1376
ν43	634.2219	1.2090	636.5760	2.0486	651.7286	50.9172
ν44	666.5728	42.6362	666.6731	45.9487	688.9584	7.1078
ν45	676.5338	2.2861	675.0670	3.3061	696.7091	10.9572
ν46	705.5329	18.0598	700.7676	17.2141	704.9196	98.3365
ν47	713.3683	51.1413	711.5930	31.7925	729.7220	117.4354
ν48	773.2060	42.1721	766.6166	54.1554	735.3563	214.1968
ν49	778.8015	82.3092	788.9930	100.9585	758.3773	12.1199
ν50	805.9114	32.7509	804.8280	16.5472	764.4107	80.3350
ν51	844.2982	73.8265	837.5185	31.5546	808.0311	19.2280
ν52	850.9793	0.5652	842.9705	46.1683	835.4293	1.6837
ν53	865.4744	100.8298	859.8872	112.6099	848.7560	24.1151
ν54	886.8240	61.8180	888.5913	56.1798	895.2612	3.3678
ν55	897.3490	5.1692	894.7168	3.6742	899.9934	12.9636
ν56	924.0775	10.8049	912.4088	23.0079	909.4951	19.3475
ν57	935.0680	16.1108	926.0317	6.9767	912.5621	68.2407
ν58	969.9830	25.1772	970.8112	28.4377	965.4501	10.7817
ν59	982.2809	0.4049	973.6345	4.0809	970.6186	0.2295
ν60	1001.3680	1.0155	994.2448	0.2072	991.5869	0.1636
ν61	1017.1413	11.2221	1015.1583	4.0110	1014.6343	2.1085
ν62	1046.1585	86.3846	1045.8428	96.6309	1041.1044	136.5774
ν63	1050.2855	179.1511	1054.4135	222.3671	1045.1686	92.9220
ν64	1076.2569	46.4964	1078.2636	57.7695	1055.7538	74.0745
ν65	1084.2857	34.4206	1083.5011	32.7163	1082.8024	147.3554
ν66	1092.5673	212.1912	1092.8973	173.1590	1096.2757	91.6443
ν67	1100.4184	34.5856	1102.0276	61.2660	1099.0954	136.8443
ν68	1107.5059	53.9226	1111.4901	31.2373	1107.9566	25.0023
ν69	1133.5663	54.9935	1133.5442	40.9685	1121.2260	80.9117
ν70	1135.1590	3.5577	1137.4248	15.6779	1130.8296	32.4485
ν71	1147.0209	92.5007	1146.5213	104.1816	1153.1904	31.2782
ν72	1162.2456	15.3048	1163.3179	17.6288	1179.3132	91.9617
ν73	1188.2899	0.4833	1188.4111	1.7611	1187.9139	1.3190
ν74	1196.2793	10.2360	1201.6370	11.9630	1203.8069	10.7925
ν75	1228.8520	63.5939	1228.6884	61.9762	1230.6761	43.3798

v76	1233.8537	53.8375	1234.1051	38.2388	1238.1632	57.0585
v77	1240.7533	187.8746	1247.8808	183.6826	1244.6587	65.6925
v78	1252.6850	76.6260	1256.3002	96.4885	1253.9379	65.9921
v79	1261.7223	37.8507	1266.7378	54.9001	1266.8771	208.0606
v80	1269.3273	37.1926	1273.5766	57.5917	1271.8833	104.5877
v81	1272.4022	25.1923	1273.8301	81.1260	1293.1218	56.4753
v82	1294.8137	35.8701	1296.3012	39.7745	1297.0662	9.6106
v83	1322.3609	3.5029	1324.1268	3.5481	1329.1531	17.3793
v84	1334.0745	1.0964	1341.2475	7.0316	1335.3800	8.2503
v85	1350.5579	41.4633	1353.3415	27.7874	1342.3691	1.4453
v86	1358.5568	15.8667	1360.4504	19.2710	1348.8940	13.4595
v87	1359.0032	0.7143	1366.0253	19.3069	1361.2149	15.9975
v88	1393.8218	5.8748	1395.7098	10.3619	1367.1804	17.3739
v89	1400.5276	2.3634	1400.7369	0.9980	1394.8220	1.8236
v90	1401.3876	1.8541	1402.0146	1.5535	1396.7148	20.6825
v91	1413.4434	25.0541	1416.1842	24.7898	1410.7249	19.6911
v92	1423.3064	14.2330	1423.6822	13.9255	1424.3148	18.3781
v93	1433.8545	55.5680	1434.9785	54.7255	1437.5620	46.0933
v94	1450.4477	34.2371	1453.1328	43.1328	1444.3819	27.1756
v95	1490.0608	30.6278	1488.6064	56.0413	1452.7053	38.0045
v96	1491.6475	44.3777	1494.0528	25.6495	1486.4816	69.7122
v97	1492.6235	2.5181	1497.7939	0.4399	1498.1131	0.4661
v98	1509.5807	15.8573	1506.6563	16.7026	1511.4020	4.8608
v99	1533.8772	69.0765	1535.0606	99.3482	1536.2386	97.8392
v100	1639.0759	7.0703	1640.2633	22.0619	1639.5011	22.7645
v101	1646.0439	35.4390	1651.6233	61.7424	1652.7243	67.5599
v102	2426.2393	410.1511	2428.4951	439.8490	2319.4912	423.6568
v103	2479.9740	312.9990	2478.9365	306.4087	2510.2535	302.2006
v104	2581.3445	225.0071	2596.4796	200.3871	2595.2772	129.8769
v105	2773.4486	57.5080	2772.5807	57.7415	2683.1362	110.1177
v106	2779.9606	54.1914	2782.3929	55.5334	2780.6066	66.8607
v107	2787.6759	79.0780	2787.8258	79.9464	2787.4600	70.6839
v108	2961.6751	22.3306	2967.8024	7.8804	2979.1362	25.8500
v109	2974.8382	32.8396	2971.7685	43.6290	2999.2513	26.8008
v110	3007.4631	31.5886	3006.7152	31.9037	3038.2191	62.5974
v111	3039.5411	50.8847	3040.0268	50.8856	3041.6600	19.2220
v112	3049.6390	52.1146	3047.5255	53.5538	3054.2460	35.4362
v113	3076.4705	18.8021	3076.8187	17.8641	3074.9471	42.3720
v114	3112.6407	35.7401	3110.3834	37.5273	3134.6559	15.5162
v115	3183.4288	0.1745	3184.9385	0.8815	3183.5289	1.4001
v116	3192.6527	12.3744	3193.1103	12.4407	3191.3393	13.6931
v117	3203.7086	25.8171	3206.0106	23.2266	3206.0982	25.7720
v118	3211.4701	11.5581	3213.4852	11.3186	3213.3803	10.8801
v119	3231.5786	0.6513	3234.9824	2.1868	3232.8508	3.7388
v120	3339.9402	867.8231	3321.1319	909.7068	3532.1236	69.0712
v121	3477.0167	655.2121	3466.5268	706.4266	3576.7526	740.5640
v122	3686.8044	107.1899	3687.8354	106.9018	3592.7597	217.8664
v123	3698.4749	50.6723	3698.5410	50.4963	3719.5044	47.9146