Supporting Information

for

The conformational behaviour of free D-glucose -at last

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Table S1. Observed frequencies and residuals (in MHz) for the rotational transitions of conformers G-g+/cc/t, G+g-/cc/t, Tg+/cc/t and G-g+/cl/g- of α-D-glucose.

						G-g+/cc/t		**G+g-/cc/t**		**Tg+/cc/t**		**G-g+/cl/g-**	
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	Obs / MHz	Obs-cal/MHz	Obs / MHz	Obs-cal/MHz	Obs / MHz	Obs-cal/MHz	Obs / MHz	Obs-cal/MHz
3	0	3	2	0	2	3884.7758	0.0027	3663.4837	0.0030	3669.27540	0.0035		
3	1	2	2	1	1	437.18010	0.0024	4187.8717	0.0009	4101.15380	0.0021		
3	1	3	2	1	2	3736.8509	0.0049	3500.1402	0.0018	3493.36650	0.0031		
3	2	2	2	2	1	4075.9266	0.0025						
4	0	4	3	0	3	5037.1523	0.0027	4723.4113	0.0013	4759.90680	0.0022		
4	1	4	3	1	3	4937.7457	0.0033	4615.6187	0.0025	4620.56920	0.0014		
4	1	3	3	1	2	5713.3028	0.0018	5487.5173	0.0020	5407.26840	0.0018		
4	2	3	3	2	2	5393.0076	0.0021	5129.6020	0.0009	5065.63760	0.0008		
4	2	2	3	2	1	5789.2298	-0.0026	5582.3512	0.0004	5403.00440	-0.0015		
4	3	2	3	3	1	5518.6963	0.0014						
5	0	5	4	0	4	6169.5517	0.0013	5762.6597	0.0006	5814.73760	0.0001		
5	1	4	4	1	3	6992.4630	-0.0006	6686.6256	-0.0031	6648.35130	-0.0009		
5	1	5	4	1	4	6117.7711	0.0010	5707.5843	0.0015	5727.62850	0.0007		
5	2	3	4	2	2	7291.4393	-0.0030	7036.1037	-0.0034	6834.69330	-0.0028		
5	3	2	4	3	1			6780.2790	-0.0018				
5	3	3	4	3	2	6902.0556	-0.0033						
5	4	2	4	4	1	6909.3900	-0.0040						
6	0	6	5	0	5	7306.9568	-0.0020	6808.2194	-0.0027	6865.47940	-0.0024		
6	1	6	5	1	5	7283.8750	-0.0032	6784.1171	-0.0019	6819.14580	-0.0022		
2	2	0	1	1	1	4655.5600	0.0034	4727.6291	0.0020				
3	1	3	2	0	2	4074.0838	0.0029	3865.7365	-0.0017	3981.75610	0.0010		
3	2	2	2	1	1	5548.9227	0.0007	5495.9837	0.0001			5579.0913	-0.0004

3	3	1	2	2	0	7023.7583	-0.0047						
4	0	4	3	1	3	4847.8454	0.0036	4521.1551	0.0026	4447.42390	0.0025	4821.3550	0.0022
4	1	4	3	0	3	5127.0522	0.0019	4817.8745	0.0008	4933.05130	0.0003	5106.5009	0.0041
5	0	5	4	1	4	6079.6521	0.0024	5668.1969	0.0015	5641.59250	0.0015	6046.3990	-0.0022
5	1	4	4	2	3	6111.0161	0.0009	5736.4322	0.0021				
5	1	5	4	0	4	6207.6713	0.0005	5802.0469	0.0004	5900.77470	0.0004	6176.8476	-0.0026
6	0	6	5	1	5	7268.8326	-0.0059	6768.8330	-0.0017	6779.44340	-0.0016		
6	1	6	5	0	5	7321.9949	-0.0037	6823.5047	-0.0017	6905.18200	-0.0028		
3	2	1	2	1	1	5792.6573	0.0019						
3	1	2	2	0	2	5303.4565	0.0035						

Table S2. Observed frequencies and residuals (in MHz) for the rotational transitions of conformers G-g+/cc/t, G+g-/cc/t and Tg+/cc/t of β-D-glucose.

						G-g+/cc/t		**G+g-/cc/t**		**Tg+/cc/t**	
J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	Obs / MHz	Obs-cal/MHz	Obs / MHz	Obs-cal/MHz	Obs / MHz	Obs-cal/MHz
3	0	3	2	0	2	3685.0790	0.0031				
3	1	2	2	1	1	4385.9599	0.0043	4198.7199	0.0020	4001.6461	0.0022
3	1	3	2	1	2						
3	2	1	2	2	0	4424.0597	0.0028	4229.7242	0.0018		
3	2	2	2	2	1	4054.5620	-0.0044	3848.8952	-0.0008		
4	0	4	3	0	3	4728.5695	0.0022	4428.8635	0.0007	4452.4104	-0.0008
4	1	4	3	1	3	4678.6378	0.0018	4373.0777	0.0000	4333.7334	0.0003
4	1	3	3	1	2	5644.4721	0.0032	5391.3902	0.0012	5240.4088	0.0016
4	2	3	3	2	2	5314.1905	0.0017	5038.0093	0.0019	4864.6636	0.0023
4	2	2	3	2	1	5984.5922	0.0009	5734.1080	0.0001	5323.4008	0.0003
4	3	2	3	3	1	5568.3933	-0.0032	5299.0298	0.0050	5009.5975	0.0056
5	0	5	4	0	4	5780.2646	0.0013	5397.0983	-0.0001	5416.5576	0.0008

5	1	4	4	1	3	6740.6739	-0.0007	6414.4703	-0.0014	6379.1956	-0.0012
5	1	5	4	1	4	5763.5250	-0.0003	5377.9049	0.0004	5354.0355	0.0002
5	2	3	4	2	2	7434.0217	-0.0034	7127.0757	-0.0030	6720.5498	-0.0008
5	3	2	4	3	1	7365.3088	-0.0042	7036.8540	-0.0026	6445.5458	-0.0004
5	3	3	4	3	2	6931.0521	-0.0010	6595.7418	-0.0020	6266.7807	-0.0048
5	4	2	4	4	1	7006.2557	-0.0030				
6	0	6	5	0	5	6842.6074	-0.0024	6376.7815	-0.0008	6386.1061	-0.0006
6	1	6	5	1	5	6837.6916	-0.0031	6371.0036	-0.0010	6357.9364	0.0003
2	2	0	1	1	1	4455.3624	0.0027	4438.1043	0.0015		
3	1	3	2	0	2	3758.4631	0.0070				
3	2	2	2	1	1	5128.2229	0.0016	5013.3102	0.0014		
3	3	1	2	2	0	6497.9817	-0.0049	6475.6089	-0.0017		
4	0	4	3	1	3	4655.1904	0.0032	4345.9273	0.0017		
4	1	4	3	0	3	4752.0174	0.0013	4456.0156	0.0007		
4	1	3	3	2	2	4902.2080	0.0048	4576.7976	-0.0005		
5	0	5	4	1	4	5756.8146	0.0001	5369.9472	0.0009		
5	1	4	4	2	3	6328.6887	-0.0002	5953.2628	0.0004		
5	1	5	4	0	4	5786.9752	0.0011	5405.0569	0.0002		
6	0	6	5	1	5	6835.8966	-0.0024	6368.8222	-0.0019		
6	1	6	5	0	5	6844.4032	-0.0024	6378.9629	0.0000		
3	2	1	2	1	1	5611.2286	0.0009				
3	1	2	2	0	2	5422.5069	0.0058				

Table S3. Cartesian coordinates for the four observed conformers of α-D-glucose. The geometries have been optimized *ab initio* at the MP2/6-311++G(d,p) level of theory.

Conformer **G-g+/cc/t:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.495021	-0.212021	-0.633301
2	6	0	0.815267	-1.500384	-0.179731
3	8	0	-0.586217	-1.402596	-0.249540
4	6	0	-1.153019	-0.308990	0.498344
5	6	0	-0.562296	1.014351	0.029394
6	6	0	0.947511	0.968563	0.152742
7	8	0	1.278311	-1.740253	1.135501
8	6	0	-2.651986	-0.399446	0.269526
9	8	0	-2.979857	-0.324578	-1.108797
10	8	0	-1.115160	2.030390	0.853565
11	8	0	1.451604	2.199735	-0.352368
12	8	0	2.909027	-0.299250	-0.523144
13	1	0	1.077839	-2.331318	-0.841960
14	1	0	-0.937408	-0.434076	1.567529
15	1	0	-0.833129	1.178070	-1.022489
16	1	0	1.209222	0.859224	1.215368
17	1	0	1.278268	-0.056911	-1.694445
18	1	0	1.008191	-2.630419	1.385218
19	1	0	3.080966	-0.672857	0.350895
20	1	0	2.410606	2.106024	-0.398194
21	1	0	-0.637486	2.838918	0.633702
22	1	0	-3.136961	0.445796	0.760357
23	1	0	-3.019654	-1.334476	0.712459
24	1	0	-2.505115	-1.047997	-1.532024

Rotational constants (GHZ): 1.2799711 0.7849445 0.5795606

Conformer **G+g-/cc/t:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.548374	-0.486400	-0.543951
2	6	0	0.491396	-1.555342	-0.279311
3	8	0	-0.801053	-1.084570	-0.577883
4	6	0	-1.182023	0.101164	0.148364
5	6	0	-0.214224	1.230229	-0.173779
6	6	0	1.191267	0.795791	0.193087
7	8	0	0.642931	-1.920496	1.078226
8	6	0	-2.606033	0.399932	-0.277466
9	8	0	-3.477569	-0.671778	0.049238
10	8	0	-0.616030	2.371205	0.567652
11	8	0	2.068934	1.856341	-0.166922
12	8	0	2.850666	-0.935738	-0.197040
13	1	0	0.640712	-2.418780	-0.935160

14	1	0	-1.159281	-0.106346	1.224985
15	1	0	-0.246491	1.437979	-1.254864
16	1	0	1.229574	0.622209	1.278328
17	1	0	1.571092	-0.277228	-1.617629
18	1	0	0.097830	-2.698137	1.239762
19	1	0	2.761777	-1.354128	0.669155
20	1	0	2.966409	1.521753	-0.051589
21	1	0	0.110399	3.002407	0.498344
22	1	0	-2.962995	1.280699	0.257640
23	1	0	-2.618862	0.607001	-1.356844
24	1	0	-3.105732	-1.449393	-0.379967

Rotational constants (GHZ): 1.3085944 0.7663058 0.5335425

Conformer **Tg+/cc/t:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.086801	-0.538760	0.029295
2	1	0	-1.052457	-0.720414	1.110634
3	6	0	-2.511466	-0.771811	-0.461266
4	1	0	-2.602293	-0.411234	-1.495899
5	1	0	-2.708222	-1.846227	-0.452183
6	8	0	-3.468687	-0.167318	0.390170
7	1	0	-3.207396	0.757833	0.475516
8	8	0	-0.253895	-1.483211	-0.662265
9	6	0	1.100970	-1.434712	-0.286224
10	1	0	1.600007	-2.171095	-0.923599
11	6	0	1.703243	-0.046555	-0.493921
12	8	0	1.299753	-1.735852	1.082140
13	1	0	1.074559	-2.662969	1.215548
14	8	0	3.054267	0.013407	-0.060091
15	1	0	1.714584	0.171188	-1.566149
16	6	0	0.849989	1.003231	0.202443
17	1	0	3.073123	-0.426491	0.799818
18	8	0	1.280993	2.319352	-0.125042
19	6	0	-0.583159	0.869062	-0.265149
20	1	0	0.883535	0.850684	1.290692
21	1	0	2.229975	2.348964	0.046079
22	8	0	-1.438375	1.795235	0.398037
23	1	0	-0.616587	1.033963	-1.353082
24	1	0	-1.017936	2.660170	0.317967

Rotational constants (GHZ): 1.3996560 0.7409966 0.5379605

Conformer **G-g+/cl/g-:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.576186	0.971338	0.005363
2	6	0	-1.113621	-0.377427	0.482154

3	8	0	-0.538942	-1.414423	-0.327691
4	6	0	0.858200	-1.505682	-0.223577
5	6	0	1.522090	-0.185567	-0.620620
6	6	0	0.929923	0.970711	0.161799
7	6	0	-2.615350	-0.515572	0.325614
8	8	0	-3.037155	-0.258991	-1.007254
9	8	0	1.198213	-1.855469	1.098181
10	8	0	2.913343	-0.330344	-0.359414
11	8	0	1.533848	2.155366	-0.345570
12	8	0	-1.072168	2.054934	0.791804
13	1	0	-0.841811	-0.528209	1.534519
14	1	0	-3.119819	0.215203	0.962109
15	1	0	-2.909386	-1.520843	0.650821
16	1	0	-2.595615	-0.915433	-1.557262
17	1	0	1.146821	-2.298665	-0.921953
18	1	0	2.135093	-1.635288	1.192226
19	1	0	1.345367	-0.013906	-1.690915
20	1	0	3.297472	0.550723	-0.443958
21	1	0	1.170599	0.851699	1.227780
22	1	0	1.103840	2.890334	0.107439
23	1	0	-0.832188	1.113976	-1.051039
24	1	0	-1.907821	2.335020	0.405381

Rotational constants (GHZ): 1.2965965 0.7877045 0.5736370

Table S4. Cartesian coordinates for the three observed conformers of β-D-glucose. The geometries have been optimized *ab initio* at the MP2/6-311++G(d,p) level of theory.

Conformer **G-g+/cc/t:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.427818	-1.383267	-0.124444
2	6	0	-0.956564	-1.268191	-0.400736
3	6	0	1.177592	-0.262663	-0.612099
4	8	0	-1.610640	-2.390309	0.107521
5	6	0	2.632835	-0.572230	-0.303302
6	1	0	1.048634	-0.165595	-1.702390
7	6	0	0.693999	1.021717	0.055128
8	8	0	1.412287	2.094313	-0.536928
9	6	0	-0.798615	1.184958	-0.160223
10	1	0	0.899615	0.963155	1.131932
11	8	0	-1.204412	2.345568	0.553252
12	1	0	-0.984490	1.321767	-1.237298
13	6	0	-1.535455	-0.053322	0.305247
14	8	0	-2.907904	0.134016	-0.009835
15	1	0	-1.389768	-0.187888	1.385970
16	1	0	-3.370306	-0.662910	0.273517
17	1	0	-2.163099	2.402338	0.465304
18	1	0	1.015639	2.902288	-0.190308
19	1	0	3.248203	0.281435	-0.591871
20	8	0	2.837740	-0.784111	1.083825
21	1	0	2.936254	-1.451362	-0.886966
22	1	0	2.240508	-1.497907	1.333692
23	1	0	-1.300078	-3.159213	-0.382336

24	1	0	-1.102985	-1.177393	-1.490471

Rotational constants (GHZ): 1.1803008 0.8197394 0.5361228

Conformer **G+g-/cc/t:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.712414	-1.132496	0.258378
2	6	0	-0.576682	-1.415215	-0.257950
3	6	0	1.215653	0.116407	-0.236558
4	8	0	-1.006012	-2.646144	0.237044
5	6	0	2.641175	0.229287	0.268095
6	1	0	1.222121	0.100789	-1.337744
7	6	0	0.321230	1.250963	0.250452
8	8	0	0.828895	2.464912	-0.279583
9	6	0	-1.102264	1.002906	-0.213485
10	1	0	0.334611	1.269524	1.350731
11	8	0	-1.909285	2.039440	0.329755
12	1	0	-1.122169	1.047021	-1.313622
13	6	0	-1.568927	-0.369746	0.226486
14	8	0	-2.860106	-0.566954	-0.331804
15	1	0	-1.598581	-0.417073	1.323815
16	1	0	-3.148750	-1.446254	-0.061972
17	1	0	-2.819423	1.840507	0.080328
18	1	0	0.154633	3.133062	-0.106517
19	1	0	3.081267	1.156402	-0.101062
20	1	0	2.625681	0.252390	1.366720
21	8	0	3.443173	-0.837729	-0.212163
22	1	0	2.997968	-1.644408	0.067916
23	1	0	-0.535140	-1.417036	-1.360207
24	1	0	-0.445962	-3.330775	-0.143636

Rotational constants (GHZ): 1.1802622 0.7933139 0.4954657

Conformer **Tg+/cc/t:**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.074981	-0.597383	-0.195879
2	1	0	1.100472	-0.593124	-1.297238
3	6	0	2.425310	-1.087308	0.315669
4	1	0	2.482251	-0.919359	1.400448
5	1	0	2.496160	-2.160919	0.127930
6	8	0	3.503541	-0.474319	-0.368379
7	1	0	3.361930	0.477732	-0.298108
8	8	0	0.081543	-1.511170	0.274961
9	6	0	-1.190877	-1.213303	-0.272444
10	8	0	-2.114248	-2.146105	0.197612
11	6	0	-1.665433	0.154341	0.195810
12	8	0	-2.897719	0.522398	-0.407074

13	1	0	-1.752632	0.123028	1.290640
14	6	0	-0.645857	1.201956	-0.202323
15	1	0	-3.539794	-0.154278	-0.163582
16	8	0	-0.944862	2.477266	0.350638
17	6	0	0.723013	0.800382	0.308804
18	1	0	-0.609012	1.265504	-1.300709
19	1	0	-1.843902	2.693993	0.077079
20	8	0	1.725857	1.706444	-0.139305
21	1	0	0.696866	0.773730	1.408229
22	1	0	1.410256	2.592052	0.078672
23	1	0	-1.124468	-1.232257	-1.373783
24	1	0	-1.837856	-3.014328	-0.115027

Rotational constants (GHZ): 1.3223546 0.7359715 0.4957015

Reference 27:

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