Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

for

Unveiling epimerization effects: a rotational study of α-D-Galactose

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Table S1. Observed frequencies and residuals (in MHz) for the rotational transitions of rotamer I.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	2	1	2	1	1	6176.327	0.019
5	1	5	4	1	4	6302.492	0.006
5	0	5	4	0	4	6376.205	0.001
5	2	4	4	2	3	6864.455	0.001
5	4	2	4	4	1	7065.326	0.012
5	3	3	4	3	2	7065.886	0.000
5	4	1	4	4	0	7071.149	0.007
5	3	2	4	3	1	7186.243	0.004
5	1	4	4	1	3	7217.960	0.015
4	1	3	3	0	3	7375.884	0.001
5	2	3	4	2	2	7447.325	0.018
6	1	6	5	1	5	7506.947	0.004
6	0	6	5	0	5	7543.780	0.006
4	2	2	3	1	2	7617.722	0.006
3	3	0	2	2	0	7655.724	0.002
3	3	1	2	2	1	7694.704	-0.006
6	2	5	5	2	4	8160.173	0.008
6	1	5	5	1	4	8471.109	0.005
6	3	4	5	3	3	8471.556	0.015
6	4	3	5	4	2	8504.542	0.004
6	4	2	5	4	1	8529.735	0.006
13	4	9	12	6	6	8604.908	-0.019
7	1	7	6	1	6	8701.955	-0.003
7	0	7	6	0	6	8718.643	-0.002
6	3	3	5	3	2	8749.703	0.025
4	3	1	3	2	1	8991.735	-0.024
4	3	2	3	2	2	9162.457	0.008
5	2	3	4	1	3	9190.621	0.009
7	2	6	6	2	5	9423.617	0.002
7	1	6	6	1	5	9649.579	0.008
7	3	5	6	3	4	9852.677	-0.018
7	6	1	6	6	0	9880.848	0.014
8	1	8	7	1	7	9891.890	0.000
8	0	8	7	0	7	9898.996	-0.001
7	5	3	6	5	2	9914.129	0.012
7	4	4	6	4	3	9948.152	-0.004
7	4	3	6	4	2	10026.431	0.014
5	3	2	4	2	2	10279.108	-0.012
7	3	4	6	3	3	10351.216	0.005
7	2	5	6	2	4	10377.462	0.006
4	4	0	3	3	0	10462.052	-0.020
4	4	1	3	3	1	10467.702	-0.021
8	2	7	7	2	6	10659.110	-0.005
8	1	7	7	1	6	10796.873	-0.017
6	2	4	5	1	4	10921.714	-0.006
9	1	9	8	1	8	11079.368	-0.005
9	0	9	8	0	8	11082.257	-0.020
8	4	4	7	4	3	11578.311	-0.017

Table S2. Observed frequencies and residuals (in MHz) for the rotational transitions of rotamer II.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	2	1	2	1	1	6035.765	0.007
5	1	5	4	0	4	6058.713	0.009
5	2	4	4	2	3	6450.413	-0.007
3	2	2	2	1	2	6451.008	0.003
5	4	2	4	4	1	6636.544	0.002
5	3	3	4	3	2	6639.705	0.005
3	2	1	2	1	2	6650.668	0.003
5	3	2	4	3	1	6745.223	0.003
5	1	4	4	1	3	6813.982	0.016
4	2	3	3	1	2	6833.882	0.004
6	0	6	5	1	5	6982.540	0.007
5	2	3	4	2	2	7010.880	0.005
6	1	6	5	1	5	7019.134	0.003
6	0	6	5	0	5	7062.924	0.002
4	1	3	3	0	3	7066.632	-0.005
6	1	5	5	2	4	7072.074	-0.002
6	1	6	5	0	5	7099.533	0.014
4	2	2	3	1	2	7377.083	0.016
3	3	1	2	2	0	7603.874	0.000
3	3	0	2	2	0	7609.383	-0.017
3	3	0	2	2	1	7651.434	0.003
6	2	5	5	2	4	7668.385	0.013
5	2	4	4	1	3	7741.828	0.016
6	3	4	5	3	3	7963.381	-0.020
6	1	5	5	1	4	7999.938	0.015
4	2	3	3	1	3	8058.169	0.003
7	0	7	6	1	6	8117.698	0.005
7	1	7	6	1	6	8133.554	0.008
7	0	7	6	0	6	8154.305	0.014
7	1	7	6	0	6	8170.154	0.010
6	3	3	5	3	2	8211.842	0.001
6	2	4	5	2	3	8437.152	0.008
7	1	6	6	2	5	8512.190	0.009
6	2	5	5	1	4	8596.221	0.002
4	2	2	3	1	3	8601.358	0.004
4	3	2	3	2	1	8824.991	-0.000
7	2	6	6	2	5	8855.211	0.017
4	3	1	3	2	1	8862.721	0.019
4	3	2	3	2	2	9024.641	-0.010
4	3	1	3	2	2	9062.367	0.005
7	1	6	6	1	5	9108.478	0.002
8	0	8	7	1	7	9235.681	0.006
8	1	8	7	1	7	9242.314	0.009
8	0	8	7	0	7	9251.535	0.007
8	1	8	7	0	7	9258.170	0.012
7	3	5	6	3	4	9265.612	0.004
7	4	4	6	4	3	9346.570	-0.001
7	4	3	6	4	2	9410.828	-0.002
7	2	6	6	1	5	9451.490	0.001
7	3	4	6	3	3	9722.343	-0.000
7	2	5	6	2	4	9797.468	0.015
8	1	7	7	2	6	9834.330	0.002
5	3	3	4	2	2	9919.420	0.008
8	2	7	7	2	6	10014.131	-0.010
8	1	7	7	1	6	10177.339	-0.001

9	0	9	8	1	8	10345.496	-0.005
9	1	9	8	1	8	10348.198	-0.004
9	0	9	8	0	8	10352.125	-0.005
9	1	9	8	0	8	10354.830	-0.002
8	2	7	7	1	6	10357.145	-0.008
4	4	1	3	3	0	10412.323	-0.005
4	4	0	3	3	0	10412.908	-0.020
4	4	1	3	3	1	10417.859	0.006
4	4	0	3	3	1	10418.449	-0.004
5	3	3	4	2	3	10462.593	-0.006
8	3	6	7	3	5	10538.076	-0.004
5	3	2	4	2	3	10605.836	0.005
8	5	4	7	5	3	10675.108	-0.023
8	5	3	7	5	2	10687.125	-0.012
6	3	4	5	2	3	10871.936	-0.003
9	1	8	8	2	7	11063.210	-0.019
8	2	6	7	2	5	11072.028	-0.010
9	2	8	8	2	7	11151.167	-0.005
8	3	5	7	3	4	11230.785	0.002
9	1	8	8	1	7	11243.030	-0.013
9	2	8	8	1	7	11330.975	-0.010
10	0	10	9	1	9	11451.681	-0.014
10	1	10	9	1	9	11452.775	0.002
10	0	10	9	0	9	11454.387	-0.009
10	1	10	9	0	9	11455.463	-0.011

Table S3. Observed frequencies and residuals (in MHz) for the rotational transitions of rotamer III.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
5	0	5	4	0	4	6062.700	0.008
5	2	4	4	2	3	6488.118	0.003
5	3	3	4	3	2	6652.008	-0.017
3	2	1	2	1	2	6702.502	0.001
5	3	2	4	3	1	6734.178	-0.005
5	1	4	4	1	3	6846.504	0.017
4	2	3	3	1	2	6977.148	0.016
5	2	3	4	2	2	6989.291	0.004
6	0	6	5	1	5	7062.198	0.020
6	1	6	5	1	5	7111.892	0.009
6	0	6	5	0	5	7165.056	0.004
6	1	6	5	0	5	7214.767	0.010
6	2	5	5	2	4	7723.825	0.009
3	3	1	2	2	0	7763.692	-0.003
3	3	0	2	2	1	7803.578	0.000
5	2	4	4	1	3	7912.382	0.004
6	3	4	5	3	3	7982.277	-0.008
6	1	5	5	1	4	8066.362	0.004
6	3	3	5	3	2	8180.424	0.007
7	0	7	6	1	6	8222.796	-0.010
7	1	7	6	1	6	8245.638	0.000
7	0	7	6	0	6	8272.513	0.002
7	1	7	6	0	6	8295.323	-0.019
6	2	4	5	2	3	8425.067	0.014
7	2	6	6	2	5	8931.676	0.010
4	3	2	3	2	1	9002.330	0.002
4	3	1	3	2	2	9202.158	0.003
7	1	6	6	1	5	9211.681	-0.006
7	3	5	6	3	4	9296.001	-0.003
7	4	4	6	4	3	9354.843	0.006
8	1	8	7	1	7	9373.200	0.004
8	0	8	7	0	7	9385.901	-0.006
7	2	6	6	1	5	9655.004	-0.009
7	3	4	6	3	3	9673.134	-0.001
7	2	5	6	2	4	9807.821	0.016
8	2	7	7	2	6	10113.461	-0.004
8	1	7	7	1	6	10308.649	-0.000
6	2	4	5	1	4	10463.454	-0.005
9	1	9	8	1	8	10497.379	-0.008
9	1	9	8	0	8	10507.512	0.005
8	3	6	7	3	5	10585.512	0.004
4	4	1	3	3	0	10630.857	0.012
4	4	0	3	3	1	10635.479	-0.002
5	3	2	4	2	3	10710.617	0.003
8	4	5	7	4	4	10712.852	-0.015
8	4	4	7	4	3	10827.879	-0.007
3	3	1	2	0	2	10905.826	-0.015
8	3	5	7	3	4	11179.762	-0.013
9	1	8	8	1	7	11392.325	-0.014

Table S4. Observed frequencies and residuals (in MHz) for the rotational transitions of rotamer IV.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	2	1	2	1	1	6147.977	-0.010
5	1	5	4	1	4	6212.162	0.012
5	0	5	4	0	4	6291.710	0.012
3	2	2	2	1	2	6552.510	0.010
5	2	4	4	2	3	6757.152	-0.011
5	3	2	4	3	1	7051.349	0.015
5	1	4	4	1	3	7110.668	-0.010
4	1	3	3	0	3	7265.406	0.007
5	2	3	4	2	2	7310.418	0.004
6	1	6	5	1	5	7400.922	0.014
6	0	6	5	0	5	7442.160	0.027
4	2	2	3	1	2	7553.333	0.006
3	3	0	2	2	0	7666.104	0.006
3	3	1	2	2	1	7702.353	0.004
6	2	5	5	2	4	8036.935	-0.000
4	2	3	3	1	3	8214.963	0.003
6	1	5	5	1	4	8356.828	0.005
6	3	3	5	3	2	8578.538	-0.017
7	1	7	6	1	6	8579.995	0.002
7	0	7	6	0	6	8599.334	0.006
6	2	4	5	2	3	8793.544	0.001
4	3	1	3	2	1	8981.498	0.001
5	2	3	4	1	3	9084.004	0.009
12	3	10	11	4	8	9665.398	-0.020
7	3	5	6	3	4	9691.622	0.011
8	1	8	7	1	7	9753.696	0.024
5	2	4	4	1	4	9963.812	-0.012
5	3	2	4	2	2	10245.617	-0.010
4	4	1	3	3	0	10479.217	-0.007
4	4	0	3	3	0	10479.831	-0.008
4	4	1	3	3	1	10484.822	0.011
5	3	3	4	2	3	10639.872	-0.013
6	2	4	5	1	4	10766.849	-0.011
9	1	9	8	1	8	10924.628	-0.017
8	2	6	7	2	5	11541.948	-0.011

Table S5. Cartesian coordinates of the observed G-g+/cl/t conformer from the optimized *ab initio* structure at the MP2/6-311++G(d,p) level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.028709	0.861964	0.546592
2	6	0	-0.486075	0.996719	0.575843
3	6	0	-1.108595	-0.398847	0.647792
4	8	0	-0.673810	-1.230441	-0.431601
5	6	0	0.717321	-1.416018	-0.475994
6	6	0	1.440060	-0.074366	-0.583039
7	6	0	-2.626178	-0.395965	0.562403
8	8	0	2.834483	-0.357635	-0.519242
9	8	0	1.675758	2.120343	0.394944
10	1	0	-0.810061	-0.846779	1.605756
11	8	0	-3.078496	0.101361	-0.698802
12	1	0	1.176399	0.382832	-1.544073
13	1	0	3.271597	0.492490	-0.384598
14	1	0	1.378864	0.449866	1.497798
15	1	0	1.166488	2.591764	-0.278468
16	8	0	-0.832366	1.734610	-0.590786
17	8	0	1.120591	-2.107176	0.686114
18	1	0	-1.750220	1.513285	-0.809404
19	1	0	-0.787029	1.551933	1.477805
20	1	0	-3.040201	0.268595	1.324982
21	1	0	-3.000855	-1.411132	0.733264
22	1	0	-2.742645	-0.517446	-1.358584
23	1	0	2.078241	-1.983007	0.739258
24	1	0	0.898687	-2.021813	-1.370330

Rotational constants (GHZ): 1.4026659 0.8030052 0.5959414

Table S6. Cartesian coordinates of the observed G+g+/cc/t conformer from the optimized *ab initio* structure at the MP2/6-311++G(d,p) level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.482217	-0.358918	0.508395
2	6	0	-0.400792	-1.432438	0.490575
3	8	0	0.879530	-0.871466	0.620468
4	6	0	1.199333	0.116451	-0.376459
5	6	0	0.188790	1.253654	-0.400985
6	6	0	-1.211883	0.678735	-0.571686
7	6	0	2.608369	0.574069	-0.047055
8	8	0	3.530842	-0.502389	-0.146934
9	8	0	-2.129967	1.761162	-0.465845
10	8	0	-2.783010	-0.916281	0.367766
11	1	0	1.202707	-0.364656	-1.363614
12	8	0	0.286230	1.990332	0.806842
13	1	0	-1.286583	0.207021	-1.561292
14	1	0	-1.457024	0.133403	1.483017
15	1	0	-2.724834	-1.542291	-0.365565
16	1	0	-2.997451	1.365759	-0.314192
17	1	0	2.922673	1.326200	-0.775215
18	1	0	2.617116	1.020972	0.952248
19	1	0	3.221709	-1.165916	0.478508
20	8	0	-0.573257	-2.137643	-0.726664
21	1	0	-0.491133	2.563460	0.820886
22	1	0	0.417468	1.897325	-1.264611
23	1	0	-0.006114	-2.915774	-0.699272
24	1	0	-0.511084	-2.104540	1.347328

Rotational constants (GHZ): 1.4039265 0.7585871 0.5548754

Table S7. Cartesian coordinates of the observed Tg+/cc/g+ conformer from the optimized *ab initio* structure at the MP2/6-311++G(d,p) level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.559364	0.075191	0.492094
2	6	0	-0.835193	0.921570	-0.542204
3	6	0	0.670374	0.828893	-0.344072
4	6	0	1.111648	-0.628034	-0.291190
5	8	0	0.339069	-1.415937	0.627310
6	6	0	-1.048017	-1.358589	0.436489
7	8	0	-1.193069	2.293886	-0.410226
8	8	0	1.065520	1.468512	0.864725
9	6	0	2.551153	-0.758578	0.208983
10	8	0	3.422610	0.147393	-0.450083
11	8	0	-1.457623	-1.867400	-0.822933
12	8	0	-2.968542	0.143596	0.311940
13	1	0	1.015909	-1.042814	-1.303045
14	1	0	-1.351558	0.473989	1.487721
15	1	0	-3.164861	-0.419462	-0.448029
16	1	0	-1.081709	0.556377	-1.548465
17	1	0	-2.150573	2.312197	-0.288936
18	1	0	0.582567	2.305468	0.881147
19	1	0	1.169329	1.301910	-1.200639
20	1	0	2.917572	-1.766795	0.004493
21	1	0	2.545807	-0.597964	1.291082
22	1	0	3.281094	1.002888	-0.030701
23	1	0	-1.294835	-2.816735	-0.821342
24	1	0	-1.476080	-1.952180	1.250244

Rotational constants (GHZ): 1.4391927 0.7593187 0.5649239

Table S8. Cartesian coordinates of the observed G-g-/cc/g+ conformer from the optimized *ab initio* structure at the MP2/6-311++G(d,p) level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.448721	-0.041532	-0.579888
2	6	0	1.007776	0.856593	0.565306
3	6	0	-0.510031	0.964182	0.581083
4	6	0	-1.129468	-0.430118	0.609750
5	8	0	-0.638178	-1.266099	-0.442294
6	6	0	0.755967	-1.395102	-0.478394
7	8	0	1.522163	2.173842	0.400802
8	8	0	-0.964305	1.663164	-0.573539
9	6	0	-2.651983	-0.422264	0.511302
10	8	0	-3.159956	-0.015409	-0.740328
11	8	0	1.285483	-2.012389	0.686483
12	8	0	2.864552	-0.169743	-0.610601
13	1	0	-0.863351	-0.870586	1.582831
14	1	0	1.155688	0.420856	-1.525133
15	1	0	3.087899	-0.793934	0.092061
16	1	0	1.345618	0.428759	1.519112
17	1	0	2.443638	2.072008	0.131415
18	1	0	-0.410326	2.451817	-0.641803
19	1	0	-0.825265	1.496783	1.490729
20	1	0	-3.026309	0.214798	1.328357
21	1	0	-3.015128	-1.439788	0.678764
22	1	0	-2.669021	0.777089	-0.989965
23	1	0	1.005805	-2.934108	0.679172
24	1	0	0.966782	-2.001182	-1.364661

Rotational constants (GHZ): 1.4073558 0.7875310 0.5882185

Complete Reference 17:

Gaussian 09 (Revision B.01), Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2010.