Supporting Information

for

Structural Expression of *Exo*-Anomeric Effect

*Elena R. Alonso, Isabel Peña, Carlos Cabezas, and José L. Alonso**

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Table S1. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
3	1	2	2	0	2	6043.041	0.001
4	1	3	3	1	2	6069.136	0.010
2	2	1	1	1	1	6128.006	-0.020
5	0	5	4	1	4	6211.510	-0.004
5	1	5	4	1	4	6385.350	0.013
5	0	5	4	0	4	6525.870	0.009
5	1	5	4	0	4	6699.680	-0.004
5	2	4	4	2	3	7023.657	0.015
3	2	2	2	1	1	7077.502	-0.012
5	4	2	4	4	1	7198.054	0.008
5	4	1	4	4	0	7200.929	0.006
3	2	1	2	1	1	7267.477	0.002
5	1	4	4	1	3	7484.768	0.014
6	0	6	5	1	5	7514.553	-0.008
6	1	6	5	1	5	7603.835	0.013
5	2	3	4	2	2	7605.757	0.009
6	0	6	5	0	5	7688.394	0.011
6	1	6	5	0	5	7777.638	-0.006
3	2	2	2	1	2	7786.531	-0.003
4	1	3	3	0	3	7996.281	-0.003
4	2	3	3	1	2	8141.359	-0.004
6	2	5	5	2	4	8359.362	0.013
6	3	4	5	3	3	8653.685	-0.004
6	4	3	5	4	2	8662.870	0.007
4	2	2	3	1	2	8672.441	0.001
6	4	2	5	4	1	8675.534	0.005
7	0	7	6	1	6	8765.162	-0.011
7	1	7	6	1	6	8808.727	0.012
6	1	5	5	1	4	8818.988	0.010
7	0	7	6	0	6	8854.446	0.012
6	3	3	5	3	2	8856.284	-0.003
7	1	7	6	0	6	8897.970	-0.005
7	1	6	6	2	5	8911.639	-0.001
5	2	4	4	1	3	9095.872	-0.008
6	2	4	5	2	3	9191.319	0.008
3	3	1	2	2	0	9525.882	0.015
3	3	0	2	2	0	9530.044	0.015
4	2	3	3	1	3	9555.234	-0.008
3	3	1	2	2	1	9565.220	0.017
7	2	6	6	2	5	9662.851	0.010
6	2	5	5	1	4	9970.465	-0.009
8	0	8	7	1	7	9984.324	-0.015
8	1	8	7	1	7	10004.813	-0.007
8	0	8	7	0	7	10027.886	0.005
8	1	8	7	0	7	10048.358	-0.004
7	1	6	6	1	5	10063.143	0.008

7	5	3	6	5	2	10096.102	-0.000
7	5	2	6	5	1	10097.646	-0.001
5	1	4	4	0	4	10133.837	-0.008
5	2	3	4	1	3	10209.050	-0.013
7	3	4	6	3	3	10481.605	-0.007
7	2	5	6	2	4	10722.922	0.012
7	2	6	6	1	5	10814.326	-0.013
4	3	1	3	2	1	10893.814	0.013
8	2	7	7	2	6	10934.988	0.011
9	1	9	8	1	8	11195.798	-0.002
9	0	9	8	0	8	11206.877	-0.026
8	1	7	7	1	6	11236.668	0.010
5	2	4	4	1	4	11430.608	-0.014
8	3	6	7	3	5	11487.623	-0.001
8	5	4	7	5	3	11570.298	-0.011
8	5	3	7	5	2	11576.332	-0.011
8	2	7	7	1	6	11686.180	-0.000
6	2	4	5	1	4	11915.603	-0.016

Table S2. Cartesian coordinates for the c- β - $^4\text{C}_1$ g- conformer. The geometries have been optimized ab initio at the MP2/6-311++G(d,p) level of theory.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.485055	-1.767278	0.206751
2	8	0.769165	-1.361925	-0.319028
3	6	1.167421	-0.086975	0.186043
4	6	0.170860	0.983317	-0.237471
5	6	-1.229247	0.582270	0.198086
6	6	-1.575013	-0.813720	-0.274800
7	8	2.399907	0.224823	-0.345643
8	8	0.544630	2.205578	0.372347
9	8	-2.118773	1.565115	-0.316706
10	8	-2.852393	-1.121899	0.286286
11	1	-1.263157	0.586609	1.299349
12	1	-0.472843	-1.777049	1.307827
13	1	0.206632	1.056988	-1.333447
14	1	-3.226708	-1.857705	-0.207399
15	1	-0.186180	2.812940	0.206989
16	1	-0.660137	-2.785526	-0.150527
17	1	-1.617894	-0.821181	-1.371458
18	1	-3.004957	1.292092	-0.052490
19	1	1.213003	-0.141942	1.290939
20	6	3.445900	-0.580651	0.188217
21	1	4.372736	-0.205160	-0.244950
22	1	3.486938	-0.480019	1.280523
23	1	3.310316	-1.632062	-0.080230
Rotational constants (MHZ):		1774.4836143	829.1320535	595.3163125

Table S3. Cartesian coordinates for the cc- β - $^4\text{C}_1$ g+ conformer. The geometries have been optimized ab initio at the MP2/6-311++G(d,p) level of theory.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.696995	-1.742581	-0.310050
2	8	-0.677503	-1.511035	-0.007228
3	6	-1.113457	-0.279527	-0.545334
4	6	-0.344152	0.874603	0.099077
5	6	1.135905	0.690768	-0.165897
6	6	1.577740	-0.673945	0.327180
7	8	-2.495692	-0.151814	-0.386493
8	8	-0.726832	2.120583	-0.467811
9	8	1.928558	1.665214	0.501816
10	8	2.919080	-0.949625	-0.039025
11	1	1.309179	0.744405	-1.251978
12	1	0.856831	-1.745326	-1.398218
13	1	-0.510315	0.871844	1.184507
14	1	3.432501	-0.178526	0.229322
15	1	-1.691249	2.132645	-0.488325
16	1	0.943316	-2.728550	0.086017
17	1	1.456456	-0.708872	1.419444
18	1	1.604237	2.527849	0.218231
19	1	-0.949573	-0.255622	-1.633089
20	6	-2.972615	-0.379504	0.943160
21	1	-4.055465	-0.270901	0.884604
22	1	-2.718450	-1.385713	1.281013
23	1	-2.576722	0.356791	1.651580
Rotational constants (MHZ):		1713.0814369	868.7174669	637.9641691

Table S4. Cartesian coordinates for the cc- β - $^4\text{C}_1$ g- conformer. The geometries have been optimized ab initio at the MP2/6-311++G(d,p) level of theory.

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.501757	-1.765569	0.165078
2	8	0.768099	-1.363015	-0.343745
3	6	1.148038	-0.108485	0.192977
4	6	0.171633	0.972445	-0.247639
5	6	-1.223613	0.605017	0.214566
6	6	-1.583903	-0.785776	-0.272908
7	8	2.398246	0.244063	-0.293799
8	8	0.485324	2.231934	0.330737
9	8	-2.206452	1.502637	-0.285792
10	8	-2.813179	-1.225859	0.280515
11	1	-1.241159	0.603474	1.315776
12	1	-0.482436	-1.820648	1.263838
13	1	0.197213	1.022815	-1.344706
14	1	-3.445400	-0.514475	0.124606
15	1	1.387724	2.438001	0.060691
16	1	-0.700632	-2.760520	-0.235327
17	1	-1.632798	-0.770807	-1.370806
18	1	-1.924261	2.388936	-0.031455
19	1	1.168026	-0.176883	1.298227
20	6	3.438425	-0.602002	0.194251
21	1	4.373317	-0.190055	-0.185043
22	1	3.451964	-0.596141	1.291513
23	1	3.308102	-1.624690	-0.167249
Rotational constants (MHZ):		1771.6144990	832.9887646	595.4016216

Table S5. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}_1$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
5	1	5	4	1	4	6375.083	-0.001
5	0	5	4	0	4	6516.161	0.004
5	2	4	4	2	3	7010.851	-0.002
5	1	4	4	1	3	7471.018	0.004
5	2	3	4	2	2	7589.159	-0.015
6	1	6	5	1	5	7591.863	0.009
6	0	6	5	0	5	7677.005	0.001
6	2	5	5	2	4	8344.582	0.013
6	3	4	5	3	3	8636.767	0.008
7	1	7	6	1	6	8795.049	0.002
6	1	5	5	1	4	8804.013	0.003
6	3	3	5	3	2	8836.904	0.001
7	0	7	6	0	6	8841.214	-0.004
6	2	4	5	2	3	9171.895	0.005
7	2	6	6	2	5	9646.294	0.006
8	1	8	7	1	7	9989.434	-0.002
8	0	8	7	0	7	10012.775	-0.015
7	1	6	6	1	5	10047.434	-0.008
7	3	5	6	3	4	10063.803	-0.001
7	3	4	6	3	3	10457.906	-0.002
7	2	5	6	2	4	10701.331	-0.005
8	2	7	7	2	6	10916.822	0.009
8	1	7	7	1	6	11220.123	-0.004

Table S6. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}_2$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	1	3	3	1	2	6066.226	0.003
5	1	5	4	1	4	6379.105	0.008
5	0	5	4	0	4	6518.216	0.005
5	2	4	4	2	3	7019.043	0.002
5	1	4	4	1	3	7479.913	0.002
6	1	6	5	1	5	7596.018	0.000
5	2	3	4	2	2	7605.002	0.005
6	0	6	5	0	5	7679.328	0.002
6	2	5	5	2	4	8353.177	-0.001
6	3	4	5	3	3	8649.859	0.010
6	1	5	5	1	4	8811.346	0.008
7	0	7	6	0	6	8844.207	-0.002
6	2	4	5	2	3	9189.403	-0.000
7	2	6	6	2	5	9654.862	-0.012
8	1	8	7	1	7	9994.007	0.000

8	0	8	7	0	7	10016.521	-0.000
7	1	6	6	1	5	10052.248	-0.004
7	3	5	6	3	4	10078.173	-0.016

Table S7. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}_3$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	1	3	3	1	2	6054.732	0.007
5	1	5	4	1	4	6371.319	0.003
5	0	5	4	0	4	6511.957	0.006
5	1	4	4	1	3	7467.423	0.003
5	2	3	4	2	2	7586.733	0.001
6	1	6	5	1	5	7587.258	0.003
6	0	6	5	0	5	7672.019	-0.001
6	2	5	5	2	4	8340.276	-0.004
7	1	7	6	1	6	8789.629	0.003
7	0	7	6	0	6	8835.530	0.003
6	2	4	5	2	3	9168.656	-0.004
7	2	6	6	2	5	9641.078	-0.006
8	1	8	7	1	7	9983.208	-0.005
8	0	8	7	0	7	10006.400	-0.001
7	1	6	6	1	5	10041.312	-0.003
7	2	5	6	2	4	10697.068	0.003

Table S8. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}_4$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	1	3	3	1	2	6044.731	0.002
5	1	5	4	1	4	6361.598	0.004
5	0	5	4	0	4	6502.324	0.004
5	2	4	4	2	3	6996.163	-0.004
5	1	4	4	1	3	7455.400	0.002
5	2	3	4	2	2	7573.507	-0.003
6	1	6	5	1	5	7575.768	-0.001
6	0	6	5	0	5	7660.692	0.003
6	2	5	5	2	4	8327.052	-0.001
7	1	7	6	1	6	8776.395	0.001
6	1	5	5	1	4	8785.511	0.003
7	0	7	6	0	6	8822.423	-0.008
6	2	4	5	2	3	9152.915	-0.003
7	2	6	6	2	5	9626.001	0.004
8	1	8	7	1	7	9968.242	0.005
8	0	8	7	0	7	9991.514	-0.004
7	1	6	6	1	5	10026.208	-0.005
7	2	5	6	2	4	10679.122	0.003

Table S9. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}_5$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	1	3	3	1	2	6058.760	0.003
5	1	5	4	1	4	6363.200	0.001
5	0	5	4	0	4	6499.231	0.006
5	2	4	4	2	3	7007.191	-0.015
5	1	4	4	1	3	7467.740	0.006
6	1	6	5	1	5	7576.203	0.007
5	2	3	4	2	2	7602.195	0.005
6	0	6	5	0	5	7656.769	0.001
6	2	5	5	2	4	8337.457	0.000
6	3	4	5	3	3	8639.593	-0.000
6	1	5	5	1	4	8792.471	0.004
6	2	4	5	2	3	9183.730	-0.005
7	2	6	6	2	5	9634.735	-0.000
7	0	7	6	0	6	8818.619	0.017
8	1	8	7	1	7	9966.588	-0.008
8	0	8	7	0	7	9987.918	-0.011
7	1	6	6	1	5	10025.673	-0.008
7	3	5	6	3	4	10064.995	0.003
8	2	7	7	2	6	10900.205	0.012

Table S10. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}_6$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
5	1	5	4	1	4	6291.054	0.001
5	0	5	4	0	4	6436.200	-0.001
5	2	4	4	2	3	6908.402	0.009
5	1	4	4	1	3	7361.489	0.004
5	2	3	4	2	2	7459.199	0.006
6	1	6	5	1	5	7493.471	-0.005
6	0	6	5	0	5	7583.072	0.002
6	2	5	5	2	4	8225.702	0.002
6	3	4	5	3	3	8502.369	0.012
7	1	7	6	1	6	8682.439	0.003
6	1	5	5	1	4	8683.508	0.001
6	3	3	5	3	2	8685.050	0.007
7	0	7	6	0	6	8732.069	-0.008
6	2	4	5	2	3	9019.129	0.001
7	2	6	6	2	5	9512.597	-0.004
8	1	8	7	1	7	9862.493	0.009
8	0	8	7	0	7	9888.110	-0.003
7	3	5	6	3	4	9909.506	-0.007
7	1	6	6	1	5	9919.781	-0.003

7	3	4	6	3	3	10272.665	-0.008
7	2	5	6	2	4	10530.789	-0.009
8	2	7	7	2	6	10769.519	0.007
9	0	9	8	0	8	11049.814	-0.005
8	1	7	7	1	6	11084.802	0.002
8	3	6	7	3	5	11294.010	-0.004

Table S11. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{18}\text{O}_1$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
5	0	5	4	0	4	6441.172	-0.006
5	2	4	4	2	3	6913.198	0.011
5	1	4	4	1	3	7366.256	-0.006
6	1	6	5	1	5	7499.387	-0.002
6	2	5	5	2	4	8231.492	0.003
6	3	3	5	3	2	8690.530	-0.004
7	2	6	6	2	5	9519.401	0.004
8	1	8	7	1	7	9870.397	-0.000

Table S12. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{18}\text{O}_2$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	1	3	3	1	2	6037.757	-0.004
5	1	5	4	1	4	6317.630	0.013
5	0	5	4	0	4	6443.900	-0.010
5	2	4	4	2	3	6973.800	0.009
6	1	6	5	1	5	7519.227	0.006
6	0	6	5	0	5	7591.487	0.008
5	2	3	4	2	2	7596.672	-0.008
6	2	5	5	2	4	8292.498	0.004
6	2	4	5	2	3	9169.237	0.003
8	0	8	7	0	7	9905.722	-0.016

Table S13. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{18}\text{O}_3$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
5	0	5	4	0	4	6420.103	0.003
5	2	4	4	2	3	6910.419	-0.010
5	1	4	4	1	3	7364.552	0.010

6	0	6	5	0	5	7563.635	-0.002
7	1	7	6	1	6	8665.660	0.003
6	1	5	5	1	4	8677.132	-0.002
7	1	6	6	1	5	9901.009	-0.003

Table S14. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{18}\text{O}_4$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
5	0	5	4	0	4	6388.364	-0.001
5	2	4	4	2	3	6859.909	0.006
5	1	4	4	1	3	7310.097	-0.009
5	2	3	4	2	2	7410.139	0.009
6	1	6	5	1	5	7438.506	0.006
6	1	5	5	1	4	8621.494	0.005
7	0	7	6	0	6	8667.132	0.008
6	2	4	5	2	3	8959.163	-0.007
8	1	8	7	1	7	9789.646	-0.012

Table S15. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{18}\text{O}_5$ monosubstituted isotopologue of conformer cc- β - $^4\text{C}_1$ g- of methyl β -D-xyloside.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{\text{obs}} - \nu_{\text{cal}}$
4	1	3	3	1	2	6047.979	0.004
5	1	5	4	1	4	6352.249	-0.002
5	0	5	4	0	4	6487.759	0.001
5	1	4	4	1	3	7454.327	-0.010
6	0	6	5	0	5	7643.379	0.011
6	2	5	5	2	4	8322.832	0.008
7	0	7	6	0	6	8803.285	-0.005
8	1	8	7	1	7	9949.474	-0.004
7	1	6	6	1	5	10007.377	-0.000

Table S16. Substitution coordinates for conformer cc- β - 4 C₁g- of methyl β -D-xylopyranoside.

atom	a	b	c
C ₁	1.1382 (14)	0.045 (34)	0.2034 (76)
C ₂	0.088 (18)	0.9664 (16)	0.2479 (64)
C ₃	1.2172 (13)	0.5987 (27)	0.2216 (72)
C ₄	1.5877 (10)	0.7754 (20)	0.2747 (57)
C ₅	0.4925 (32)	1.77026 (90)	0.1645 (98)
C ₆	3.44875 (45)	0.5995 (26)	0.1930 (80)
O ₁	2.39812 (64)	0.2225 (70)	0.2965 (52)
O ₂	0.4974 (34)	2.23155 (75)	0.3137 (54)
O ₃	2.20226 (73)	1.5113 (11)	0.2780 (58)
O ₄	2.81852 (57)	1.2210 (13)	0.2730 (59)
O ₅	0.7529 (20)	1.3626 (11)	0.3415 (45)

^aPrincipal inertial axis coordinates in Å; derived errors in parentheses in units of the last digit; These were calculated according to Constains formula: $\sigma(x) = K/|x|$; $\sigma(x)$ is the error in the x coordinate and $K = 0.0012 \text{ Å}^2$.

Table S17. Experimental results of methyl β -D-xyloside and comparison with theoretical predictions.

	Experimental	MP2/B3LYP/M06HF/M05-2X /M06-2X 6-311++G(d,p)	MP2/B3LYP/M06HF/M05-2X /M06-2X cc-pVTZ	MP2/B3LYP/M06HF/M05-2X /M06-2X Aug-cc-pVTZ
A ^a / MHz	1766.25692 (72) ^c	1771.6/1756.3/1779.0/1783.3/1779.3	1782.7/1765.4/1782.9/1790.2/1785.5	1777.8/1762.0/1781.9/1788.1/1783.6
B/ MHz	829.25439 (24)	833.0/ 820.0/834.9/835.6/835.2	837.4/822.7/836.1/837.8/837.2	835.4/821.2/835.2/836.7/836.2
C/ MHz	592.91443 (17)	595.4/586.9/595.8/597.1/596.2	598.6/589.2/597.0/598.9/597.8	597.2/588.1/596.4/598.1/597.0
r(C ₁ -O ₁) ^b /Å	1.3816 (77)	1.387/1.389/1.382/1.384/1.382	1.385/1.388/1.382/1.384/1.382	1.386/1.388/1.381/1.383/1.381

^aA, B and C are the rotational constants. ^b C₁-O₁ bond distance. ^cStandard error in parentheses in units of the last digit.

Complete Reference 30:

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