Supplementary Information

for

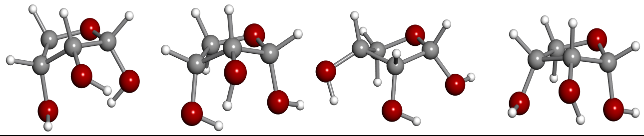
Erythrose revealed as furanose forms

Carlos Cabezas, Isabel Peña, Adam M. Daly, and José L. Alonso

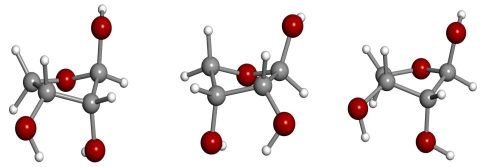
Contents

Table S1. Calculated spectroscopic parameters and ab initio energies at the MP2/6-311++G(d,p) level of theory for the lowest-energy α- and ß-furanoside conformers of erythrose.

	α-^{2}E-cc	**α-^{2}E-c**	**α-^{3}T$_{4}$-cc**	**α-^{0}T$_{1}$-cc**
A[a]/MHz	2609.2	2626.9	3351.6	2590.7
B/MHz	2346.7	2263.1	1964.1	2354.0
C/MHz	1788.8	1814.4	1447.3	1677.8
μ_a/D	0.30	-2.16	2.52	-1.02
μ_b/D	-1.90	-0.52	0.78	-0.21
μ_c/D	-1.33	0.05	0.26	-0.70
ΔE[b]/cm^{-1}	0	167	453	640



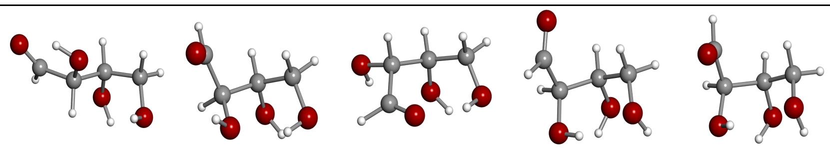
	β-^{1}T$_{2}$-cc	**β-^{4}E-c**	**β-E$_{2}$-cc**
A[a]/MHz	3107.3	2958.7	3122.0
B/MHz	1865.0	2102.8	1814.0
C/MHz	1642.2	1470.9	1607.3
μ_a/D	2.23	-0.61	-1.56
μ_b/D	-0.14	-2.33	1.83
μ_c/D	1.11	-0.15	-0.66
ΔE[b]/cm^{-1}	816	885	1004



[a] A, B and C are the rotational constants; μ_a, μ_b and μ_c are the electric dipole moment components. [b]MP2/6-311++G(d,p) electronic energies respect to the global minimun.

Table S2. Calculated spectroscopic parameters and relative energies for the lowest-energy conformers of linear forms of erythrose from ab initio computations.

	linear-1	**linear-2**	**linear-3**	**linear-4**	**linear-5**
A[a]/MHz	3594.7	3246.7	2601.3	2641.9	2795.0
B/MHz	1363.9	1423.1	1885.2	1575.2	1682.5
C/MHz	1101.3	1295.8	1329.7	1472.1	1438.7
μ_a/D	0.90	1.53	0.83	-1.43	1.34
μ_b/D	-0.27	1.43	-0.27	0.21	-0.71
μ_c/D	-0.50	-1.36	1.32	0.86	-2.59
ΔE[b]/cm^{-1}	1702	1875	2243	2441	2604



[a] A, B and C are the rotational constants; μ_a, μ_b and μ_c are the electric dipole moment components. [b]MP2/6-311++G(d,p) electronic energies respect to the global minimun.

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

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
2	1	2	1	0	1	7906.6077	0.0100
2	0	2	1	1	1	7615.1374	0.0016
2	2	1	1	1	0	9533.9394	0.0041
2	1	1	1	0	1	9646.1763	0.0031
2	2	0	1	1	0	9937.6351	0.0000
2	2	1	1	1	1	10113.7863	-0.0074
3	0	3	2	1	2	11294.4348	-0.0074
3	1	3	2	0	2	11361.3085	-0.0014

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

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	$\nu_{obs.}$	$\nu_{obs.}-\nu_{cal.}$
2	1	2	1	1	1	6705.7910	-0.0037
2	0	2	1	0	1	6914.1901	-0.0003
2	1	1	1	1	0	7184.9436	0.0002
2	1	1	1	0	1	8677.5875	-0.0017
3	1	3	2	1	2	10040.3326	0.0053
3	0	3	2	0	2	10296.7123	0.0211
3	1	2	2	1	1	10756.4858	-0.0025

Table S5. Cartesian coordinates for the three low-energy conformers of D-erythrose. The geometries have been optimized *ab initio* at the MP2/6-311++G(d,p) level of theory.

Conformer α-^{2}E-cc

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.709955	-0.319883	-0.231547
2	6	0	0.435195	-1.142532	-0.229508
3	6	0	-0.556357	-0.163461	-0.866271
4	6	0	-0.091864	1.173003	-0.260415
5	8	0	1.305921	1.065054	-0.160277
6	8	0	0.063954	-1.394802	1.124123
7	8	0	-1.902454	-0.477474	-0.583226
8	8	0	-0.714463	1.406201	0.984456
9	1	0	-0.332510	2.043297	-0.872834
10	1	0	2.339762	-0.553414	0.629759
11	1	0	-0.408363	-0.142900	-1.951770
12	1	0	-2.182103	0.162461	0.086192
13	1	0	-0.394651	0.707992	1.574906
14	1	0	0.534485	-2.079147	-0.788414
15	1	0	-0.837151	-1.741166	1.084857
16	1	0	2.275301	-0.471723	-1.156852

Conformer ß-$^1T_2$-cc

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.126727	-1.316039	0.621966
2	6	0	-0.790470	-0.555952	-0.552703
3	6	0	-0.146087	0.836283	-0.435918
4	6	0	1.225838	0.469711	0.095753
5	8	0	0.939746	-0.465695	1.117654
6	8	0	-2.200141	-0.518089	-0.497570
7	8	0	-0.851749	1.624375	0.517520
8	8	0	1.948310	-0.096523	-0.969534
9	1	0	-0.834265	-1.470385	1.439643
10	1	0	-0.126072	1.394117	-1.371153
11	1	0	-0.591216	1.304310	1.391086
12	1	0	2.767806	-0.443557	-0.600065
13	1	0	1.763590	1.297024	0.568248
14	1	0	0.289945	-2.277403	0.311508
15	1	0	-0.515397	-1.010378	-1.505564
16	1	0	-2.419044	0.249712	0.047152

Complete Reference 19:

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.