Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

for

Conformations of D-Xylose: The pivotal role of the intramolecular hydrogen-bonding

Table S1. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer cc α $^4C_1$ of D-xylose.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
2	2	1	1	1	1	6502.610	0.005
3	2	2	2	2	1	6590.751	0.005
2	2	0	1	1	1	6739.394	0.003
3	1	2	2	1	1	7075.989	0.004
2	2	0	1	0	1	7132.376	0.005
3	2	1	2	2	0	7295.555	0.002
4	1	3	3	2	1	7353.782	0.001
4	0	4	3	1	3	7532.298	0.007
4	1	4	3	1	3	7543.763	0.008
4	0	4	3	0	3	7580.306	0.008
4	1	4	3	0	3	7591.774	0.011
3	2	2	2	1	1	7769.689	0.004
4	1	3	3	2	2	8295.380	0.007
4	2	3	3	2	2	8591.209	0.003
3	1	2	2	0	2	8635.588	0.003
3	2	1	2	1	1	8711.279	0.001
4	1	3	3	1	2	8989.075	0.001
4	3	2	3	3	1	9101.732	0.002
3	2	2	2	1	2	9164.444	0.005
4	2	3	3	1	2	9284.905	-0.001
5	0	5	4	1	4	9285.953	0.006
5	1	5	4	1	4	9288.413	0.004
5	0	5	4	0	4	9297.414	0.002
5	1	5	4	0	4	9299.873	-0.000
4	3	1	3	3	0	9516.075	-0.008
3	3	1	2	2	0	9605.429	0.005
3	3	0	2	2	0	9693.289	-0.003
4	2	2	3	2	1	9771.780	-0.006
3	3	1	2	2	1	9842.210	0.000
3	3	0	2	2	1	9930.074	-0.004
3	2	1	2	1	2	10106.035	0.004
3	2	1	2	0	2	10270.878	-0.000
5	2	4	4	2	3	10470.672	-0.003
5	1	4	4	1	3	10671.674	-0.003
5	2	4	4	1	3	10766.485	-0.022
6	0	6	5	1	5	11022.857	-0.005
6	1	6	5	1	5	11023.353	-0.004
6	0	6	5	0	5	11025.321	-0.002
6	1	6	5	0	5	11025.819	0.001
3	3	0	2	1	1	11109.013	-0.003
5	3	3	4	3	2	11269.587	-0.012

Table S2. Observed frequencies and residuals (in MHz) for the rotational transitions of conformer c α $^4C_1$ of D-xylose.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
2	2	1	1	1	1	6515.249	-0.001
3	2	2	2	2	1	6625.561	0.005

2	2	0	1	1	1	6756.113	-0.000
3	1	2	2	1	1	7110.470	0.002
2	2	0	1	0	1	7143.596	-0.004
3	2	1	2	2	0	7339.187	0.000
4	0	4	3	0	3	7615.220	0.010
4	2	3	3	2	2	8633.955	0.001
3	2	1	2	1	1	8742.509	0.002
4	1	3	3	1	2	9026.844	-0.000
4	3	2	3	3	1	9152.372	-0.007
3	2	2	2	1	2	9191.640	-0.006
5	1	5	4	1	4	9332.894	0.004
5	0	5	4	0	4	9341.436	0.013
4	3	1	3	3	0	9577.062	0.003
4	2	2	3	2	1	9824.786	-0.010
3	2	1	2	0	2	10306.618	0.006
5	2	4	4	2	3	10520.133	0.009
5	1	4	4	1	3	10715.028	0.004
6	1	6	5	1	5	11076.315	-0.015
6	0	6	5	0	5	11078.154	-0.011

Table S3. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}C_1$ monosubstituted isotopologue of conformer cc α $^4C_1$ of D-xylose.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	2	2	2	2	1	6555.979	-0.006
3	1	2	2	1	1	7040.478	0.001
3	2	1	2	2	0	7249.941	0.002
4	1	4	3	1	3	7510.780	0.001
4	0	4	3	0	3	7548.723	0.001

Table S4. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}C_2$ monosubstituted isotopologue of conformer cc α $^4C_1$ of D-xylose.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	2	2	2	2	1	6576.340	-0.007
3	2	1	2	2	0	7279.272	0.004
4	1	4	3	1	3	7528.123	-0.006
4	0	4	3	0	3	7564.501	0.008
5	1	5	4	1	4	9269.294	0.000

Table S5. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}C_3$ monosubstituted isotopologue of conformer cc α $^4C_1$ of D-xylose.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	2	2	2	2	1	6583.535	0.016
3	2	1	2	2	0	7290.026	-0.004
4	1	4	3	1	3	7532.948	-0.008

4	0	4	3	0	3	7568.970	0.001
4	2	3	3	2	2	8580.682	-0.007
5	0	5	4	0	4	9283.710	0.004

Table S6. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}C_4$ monosubstituted isotopologue of conformer cc α $^4C_1$ of D-xylose.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	2	2	2	2	1	6560.364	0.000
3	1	2	2	1	1	7045.279	0.000
3	2	1	2	2	0	7254.231	-0.001
4	1	4	3	1	3	7516.360	0.006
4	0	4	3	0	3	7554.434	-0.001
4	1	3	3	1	2	8958.021	-0.000
5	1	5	4	1	4	9255.304	-0.004

Table S7. Observed frequencies and residuals (in MHz) for the rotational transitions of $^{13}C_5$ monosubstituted isotopologue of conformer cc α $^4C_1$ of D-xylose.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	ν_{obs}	$\nu_{obs} - \nu_{cal}$
3	2	2	2	2	1	6572.087	0.002
3	1	2	2	1	1	7053.066	-0.001
3	2	1	2	2	0	7291.549	0.001
4	1	4	3	1	3	7505.032	-0.006
4	0	4	3	0	3	7538.385	0.007
4	2	3	3	2	2	8559.499	-0.001
5	0	5	4	0	4	9247.073	-0.000

Table S8. Rotational parameters of the monosubstituted isotopologues of conformer cc α $^4C_1$ of D-xylose.

Parameter	**^{13}C(1)**	**^{13}C(2)**	**^{13}C(3)**	**^{13}C(4)**	**^{13}C(5)**
A /MHz[a]	1721.1371(79)[d]	1719.297(41)	1720.169(34)	1722.7058(32)	1707.5224(76)
B /MHz	1323.06599(84)	1327.8312(43)	1329.7876(34)	1323.87715(57)	1329.45972(78)
C /MHz	862.26212(70)	864.2846(24)	864.7186(23)	862.91080(38)	861.23530(57)
σ[b] / KHz	2.7	5.6	8.3	2.9	3.6
N[c]	5	5	6	7	7

[a] A, B and C are the rotational constants. [b] Rms deviation of the fit. [c] Number of fitted transitions. [d] Standard error in parenthesis in the units of the last digit.

Table S9. Substitution coordinates of conformer cc α $^4C_1$ of D-xylose (principal-inertial-axis coordinates in Å); *ab initio* data according to MP2/6-311++G(d,p).

	Substitution Coordinates			***MP2 Coordinates***		
Atom	/a/	/b/	/c/	*a*	*b*	*c*
C_1	1.46736(82)	0.6191(19)	0.3136(38)	1.46252	-0.62357	-0.32401
C_2	0.7908(17)	0.7312(16)	0.5066(24)	0.80242	0.74153	-0.50772
C_3	0.5239(23)	0.7695(16)	0.2172(55)	-0.54196	0.77621	0.20369
C_4	1.39834(86)	0.3733(32)	0.2596(46)	-1.39636	-0.38407	-0.26535
C_5	0.6357(19)	1. 68354(71)	0.014(86)	-0.64082	-1.68141	-0.02147