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DOI: <https://doi.org/10.1016/j.jms.2020.111374>

## **Investigation of the Rotamers of 3-Furfural by Microwave Spectroscopy**

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**Appendix I: Equilibrium (B3LYP-D3(BJ)/aug-cc-pVTZ) and literature ground state spectroscopic constants**

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## Appendix I: Equilibrium (B3LYP-D3(BJ)/aug-cc-pVTZ) and literature ground state spectroscopic constants

Table S1: Equilibrium spectroscopic constants (B3LYP-D3(BJ)/aug-cc-pVTZ)(this work)<sup>a</sup> and ground state constants reported in ref 13<sup>b</sup> for 3-furfural (3-FF)

	<i>anti</i> -3-FF <sup>a</sup>	<i>syn</i> -3-FF <sup>a</sup>	<i>anti</i> -3-FF <sup>b</sup>
Rotational Constants /MHz			
A	8282.3	8223.0	8238.7276(16)
B	1983.0	1990.9	1976.13883(42)
C	1599.9	1602.8	1593.97114(34)
Centrifugal Distortion Constants /kHz			
$\Delta_J$	0.1340	0.1396	0.13902(89)
$\Delta_{JK}$	0.5615	0.6123	0.7482(92)
$\Delta_K$	2.005	1.808	1.7616(89)
$\delta_J$	0.03049	0.03166	0.03099(17)
$\delta_K$	0.7650	0.7882	0.829(14)
Sextic Centrifugal Distortion Constants /Hz			
$\Phi_{JK}$			-0.001331(45)
no. of lines	-	-	239
rms /MHz	-	-	0.046

## Appendix II: Equilibrium Structures from B3LYP-D3(BJ)/aug-cc-pVTZ

Table S2: Z-matrix structure for *anti*-3-furfural.

O1						
C2	1			1.3476147		
C3	2	1		1.3654363	110.4710932	
C4	3	2	1	1.4381344	106.0111748	0.0015286
C5	4	3	2	1.3487330	106.0858748	0.0040830
C6	3	4	5	1.4563540	128.2295757	-179.9963108
O7	6	3	4	1.2114324	124.4127059	-0.0308925
H8	6	3	4	1.1072730	114.9065594	179.9711021
H9	2	3	4	1.0753804	132.9047653	-179.9993759
H10	4	5	1	1.0750104	127.6398597	179.9960227
H11	5	4	3	1.0740305	134.0427382	179.9982408

Table S3: Z-matrix structure for *syn*-3-furfural.

O1						
C2	1			1.3471198		
C3	2	1		1.3658406	110.3111591	
C4	3	2	1	1.4384051	105.8951122	0.0039864
C5	4	3	2	1.3505592	106.2834220	-0.0155861
C6	3	4	5	1.4603413	127.3597456	179.9909142
O7	6	3	4	1.2113517	124.7679229	179.9553334
H8	6	3	4	1.1072665	114.6949431	-0.0382961
H9	2	3	4	1.0742074	132.5302331	-179.9945191
H10	4	5	1	1.0761759	126.6848154	-179.9894812
H11	5	4	3	1.0738432	134.1316705	-179.9939883

**Appendix III: Assigned Transitions for 3-furfural**Table S4: *anti*-3-furfural (parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
1	1	0	1	0	1	6644.7541	6644.7539	0.0002
2	1	2	1	1	1	6758.0521	6758.0521	0.0000
2	1	1	2	0	2	7043.8761	7043.8761	0.0000
2	0	2	1	0	1	7123.2573	7123.2573	0.0000
2	1	1	1	1	0	7522.3800	7522.3795	0.0005
3	1	2	3	0	3	7673.8936	7673.8935	0.0001
6	1	5	6	1	6	7986.0578	7986.0578	0.0000
4	1	3	4	0	4	8570.4687	8570.4686	0.0000
4	0	4	3	1	3	8731.3918	8731.3923	-0.0004
5	1	4	5	0	5	9776.1467	9776.1466	0.0001
2	2	0	3	1	3	9824.4945	9824.4954	-0.0009
1	1	1	0	0	0	9832.7004	9832.7005	0.0000
3	1	3	2	1	2	10126.6965	10126.6968	-0.0002
7	1	6	7	1	7	10602.7699	10602.7697	0.0001
3	0	3	2	0	2	10642.6953	10642.6958	-0.0005
3	2	2	2	2	1	10710.3033	10710.3021	0.0011
3	2	1	2	2	0	10777.9267	10777.9260	0.0007
3	1	2	2	1	1	11272.7128	11272.7132	-0.0004
6	1	5	6	0	6	11333.3833	11333.3832	0.0000
5	0	5	4	1	4	12768.7909	12768.7909	0.0000
2	1	2	1	0	1	13020.6415	13020.6415	0.0000
7	1	6	7	0	7	13274.7926	13274.7927	0.0000
4	1	4	3	1	3	13483.5318	13483.5320	-0.0002
8	1	7	8	1	8	13544.7076	13544.7075	0.0000
4	0	4	3	0	3	14112.7773	14112.7774	-0.0001

4	2	3	3	2	2	14267.1902	14267.1904	-0.0001
4	3	2	3	3	1	14312.9091	14312.9090	0.0001
4	3	1	3	3	0	14315.7316	14315.7316	0.0000
4	2	2	3	2	1	14434.8124	14434.8127	-0.0002
4	1	3	3	1	2	15009.3525	15009.3525	0.0000
4	1	3	3	1	2	15009.3525	15009.3525	0.0000
8	1	7	8	0	8	15613.1183	15613.1185	-0.0002
3	1	3	2	0	2	16024.0806	16024.0809	-0.0003
8	2	6	8	1	7	16147.0072	16147.0074	-0.0001
7	2	5	7	1	6	16276.4602	16276.4603	0.0000
6	2	4	6	1	5	16637.0613	16637.0612	0.0001
6	0	6	5	1	5	16803.7130	16803.7126	0.0004
5	1	5	4	1	4	16825.6685	16825.6684	0.0000
5	2	3	5	1	4	17151.0144	17151.0139	0.0004
5	0	5	4	0	4	17520.9309	17520.9307	0.0002
4	2	2	4	1	3	17735.3737	17735.3732	0.0005
5	2	4	4	2	3	17812.7788	17812.7788	0.0000
5	4	2	4	4	1	17888.0507	17888.0508	-0.0001
5	4	1	4	4	0	17888.1374	17888.1375	-0.0001
5	3	3	4	3	2	17903.9267	17903.9268	-0.0001
5	3	2	4	3	1	17913.7789	17913.7792	-0.0003
5	2	3	4	2	2	18142.2492	18142.2493	-0.0001
3	2	1	3	1	2	18309.9133	18309.9130	0.0003
5	1	4	4	1	3	18726.6089	18726.6086	0.0002
2	2	0	2	1	1	18804.6997	18804.7002	-0.0004
4	1	4	3	0	3	18864.9169	18864.9171	-0.0002

Table S5: *anti*-3-furfural ( $^{18}\text{O}1$ )

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
2	1	2	1	1	1	6587.8418	6587.8436	-0.0018
1	1	0	1	0	1	6627.0603	6627.0603	0.0000
2	0	2	1	0	1	6937.3526	6937.3550	-0.0023
2	1	1	2	0	2	7007.5562	7007.5559	0.0003
2	1	1	1	1	0	7317.8502	7317.8506	-0.0004
3	1	2	3	0	3	7606.9522	7606.9521	0.0000
4	0	4	3	1	3	8335.0386	8335.0381	0.0004
4	1	3	4	0	4	8457.9837	8457.9844	-0.0007
5	1	4	5	0	5	9600.0512	9600.0518	-0.0006
1	1	1	0	0	0	9738.4834	9738.4827	0.0007
3	1	3	2	1	2	9872.2725	9872.2730	-0.0005
3	0	3	2	0	2	10367.4725	10367.4726	0.0000
3	2	2	2	2	1	10429.2518	10429.2499	0.0018
3	2	1	2	2	0	10491.0458	10491.0449	0.0009

3	1	2	2	1	1	10966.8686	10966.8687	-0.0001
6	1	5	6	0	6	11073.2467	11073.2465	0.0001
5	0	5	4	1	4	12269.4450	12269.4447	0.0003
2	1	2	1	0	1	12849.9013	12849.8997	0.0015
4	1	4	3	1	3	13145.8780	13145.8784	-0.0003
4	0	4	3	0	3	13752.3831	13752.3833	-0.0001
4	2	3	3	2	2	13893.5979	13893.5971	0.0007
4	3	2	3	3	1	13935.4134	13935.4129	0.0005
4	3	1	3	3	0	13937.8783	13937.8793	-0.0009
4	2	2	3	2	1	14046.8814	14046.8808	0.0006
4	1	3	3	1	2	14603.4160	14603.4156	0.0004
3	1	3	2	0	2	15784.8179	15784.8178	0.0000
6	0	6	5	1	5	16207.9758	16207.9755	0.0003
5	1	5	4	1	4	16405.9684	16405.9689	-0.0005
5	0	5	4	0	4	17080.2847	17080.2849	-0.0002
5	2	4	4	2	3	17347.6197	17347.6201	-0.0004
5	3	3	4	3	2	17431.0718	17431.0705	0.0013
5	3	2	4	3	1	17439.6806	17439.6817	-0.0011
5	2	3	4	2	2	17649.3347	17649.3352	-0.0004
5	1	4	4	1	3	18222.3521	18222.3524	-0.0002
4	1	4	3	0	3	18563.2231	18563.2236	-0.0004

Table S6: *anti*-3-furfural ( $^{13}\text{C}_2$ )

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
1	1	0	1	0	1	6496.3379	6496.3402	-0.0023
2	1	2	1	1	1	6727.9796	6727.9803	-0.0006
2	1	1	2	0	2	6900.7961	6900.7984	-0.0022
2	0	2	1	0	1	7096.8861	7096.8863	-0.0002
2	1	1	1	1	0	7501.3452	7501.3445	0.0007
3	1	2	3	0	3	7540.3033	7540.3042	-0.0008
4	1	3	4	0	4	8452.0888	8452.0881	0.0006
4	0	4	3	1	3	8833.0132	8833.0139	-0.0006
1	1	1	0	0	0	9666.9928	9666.9918	0.0010
5	1	4	5	0	5	9680.2309	9680.2306	0.0003
3	1	3	2	1	2	10081.0975	10081.0973	0.0001
3	0	3	2	0	2	10601.1236	10601.1232	0.0004
3	2	2	2	2	1	10671.9694	10671.9721	-0.0027
3	1	2	2	1	1	11240.6307	11240.6290	0.0017
6	1	5	6	0	6	11267.9767	11267.9773	-0.0005
2	1	2	1	0	1	12837.6394	12837.6378	0.0015
5	0	5	4	1	4	12853.0119	12853.0118	0.0001
4	1	4	3	1	3	13421.8697	13421.8700	-0.0003
4	0	4	3	0	3	14053.7393	14053.7396	-0.0002

4	2	3	3	2	2	14215.4485	14215.4481	0.0003
4	3	1	3	3	0	14266.3867	14266.3868	-0.0001
4	2	2	3	2	1	14391.0033	14391.0022	0.0011
4	1	3	3	1	2	14965.5245	14965.5235	0.0010
3	1	3	2	0	2	15821.8493	15821.8488	0.0004
5	2	3	5	1	4	16696.1266	16696.1263	0.0003
5	1	5	4	1	4	16747.3175	16747.3182	-0.0006
6	0	6	5	1	5	16864.9726	16864.9712	0.0013
4	2	2	4	1	3	17274.4102	17274.4107	-0.0004
5	0	5	4	0	4	17441.8668	17441.8678	-0.0010
5	2	4	4	2	3	17747.0819	17747.0824	-0.0005
5	3	3	4	3	2	17842.4496	17842.4501	-0.0004
3	2	1	3	1	2	17848.9334	17848.9320	0.0013
5	3	2	4	3	1	17853.1480	17853.1467	0.0012
5	2	3	4	2	2	18091.7254	18091.7259	-0.0004
4	1	4	3	0	3	18642.5945	18642.5956	-0.0011
5	1	4	4	1	3	18670.0095	18670.0103	-0.0007

Table S7: *anti*-3-furfural ( $^{13}\text{C}$ 3)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{\text{obs}}$ /MHz	$\nu_{\text{calc}}$ /MHz	$\nu_{\text{obs-calc}}$ /MHz
1	1	0	1	0	1	6640.8219	6640.8228	-0.0009
2	1	2	1	1	1	6756.1043	6756.1052	-0.0008
2	1	1	2	0	2	7039.9397	7039.9398	0.0000
2	0	2	1	0	1	7121.2884	7121.2871	0.0013
2	1	1	1	1	0	7520.4041	7520.4041	0.0000
3	1	2	3	0	3	7669.9658	7669.9657	0.0000
4	1	3	4	0	4	8566.5798	8566.5798	0.0000
5	1	4	5	0	5	9772.3419	9772.3420	0.0000
1	1	1	0	0	0	9827.8037	9827.8031	0.0006
3	1	3	2	1	2	10123.7707	10123.7711	-0.0004
7	1	6	6	2	5	10583.8530	10583.8528	0.0001
3	0	3	2	0	2	10639.7179	10639.7183	-0.0003
3	2	2	2	2	1	10707.3609	10707.3606	0.0002
3	2	1	2	2	0	10775.0210	10775.0204	0.0006
3	1	2	2	1	1	11269.7441	11269.7442	-0.0001
6	1	5	6	0	6	11329.7123	11329.7118	0.0005
5	0	5	4	1	4	12767.4657	12767.4657	0.0000
2	1	2	1	0	1	13014.7777	13014.7778	0.0000
7	1	6	7	0	7	13271.2851	13271.2853	-0.0002
4	1	4	3	1	3	13479.6217	13479.6219	-0.0002
4	0	4	3	0	3	14108.7680	14108.7681	0.0000
4	2	3	3	2	2	14263.2621	14263.2615	0.0006
4	3	2	3	3	1	14309.0049	14309.0043	0.0005

4	3	1	3	3	0	14311.8298	14311.8300	-0.0002
4	2	2	3	2	1	14430.9709	14430.9711	-0.0001
4	1	3	3	1	2	15005.3817	15005.3821	-0.0004
3	1	3	2	0	2	16017.2618	16017.2619	0.0000
7	2	5	7	1	6	16265.9873	16265.9877	-0.0004
6	2	4	6	1	5	16626.0912	16626.0907	0.0004
6	0	6	5	1	5	16801.1425	16801.1423	0.0002
5	1	5	4	1	4	16820.7674	16820.7674	0.0000
5	2	3	5	1	4	17139.6904	17139.6903	0.0001
5	0	5	4	0	4	17515.8631	17515.8631	0.0000
4	2	2	4	1	3	17723.8241	17723.8232	0.0009
5	2	4	4	2	3	17807.8564	17807.8565	0.0000
5	3	3	4	3	2	17899.0510	17899.0513	-0.0003
5	3	2	4	3	1	17908.9140	17908.9146	-0.0006
5	2	3	4	2	2	18137.4923	18137.4924	0.0000
3	2	1	3	1	2	18298.2347	18298.2343	0.0004
5	1	4	4	1	3	18721.6253	18721.6253	0.0000
2	2	0	2	1	1	18792.9566	18792.9581	-0.0014
4	1	4	3	0	3	18857.1659	18857.1655	0.0004

Table S8: *anti*-3-furfural ( $^{13}\text{C4}$ )

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
1	1	0	1	0	1	6490.4258	6490.4256	0.0001
2	1	2	1	1	1	6737.1841	6737.1840	0.0001
2	1	1	2	0	2	6896.3326	6896.3321	0.0004
2	0	2	1	0	1	7107.2600	7107.2601	-0.0001
2	1	1	1	1	0	7513.1669	7513.1666	0.0002
3	1	2	3	0	3	7538.2627	7538.2637	-0.0009
4	1	3	4	0	4	8453.7220	8453.7221	-0.0001
4	0	4	3	1	3	8862.5728	8862.5734	-0.0005
1	1	1	0	0	0	9665.0261	9665.0244	0.0017
5	1	4	5	0	5	9687.0644	9687.0652	-0.0007
3	1	3	2	1	2	10094.8179	10094.8186	-0.0006
3	0	3	2	0	2	10616.3389	10616.3398	-0.0008
3	2	2	2	2	1	10687.7403	10687.7409	-0.0006
3	2	1	2	2	0	10759.1600	10759.1604	-0.0003
3	1	2	2	1	1	11258.2723	11258.2713	0.0009
6	1	5	6	0	6	11281.7134	11281.7136	-0.0001
2	1	2	1	0	1	12839.6187	12839.6175	0.0011
7	1	6	7	0	7	13269.4742	13269.4745	-0.0002
4	1	4	3	1	3	13440.0155	13440.0163	-0.0008
4	0	4	3	0	3	14073.4094	14073.4096	-0.0001
4	2	3	3	2	2	14236.3640	14236.3642	-0.0001

4	3	2	3	3	1	14284.6061	14284.6056	0.0005
4	3	1	3	3	0	14287.7088	14287.7083	0.0005
4	2	2	3	2	1	14413.2731	14413.2721	0.0010
4	1	3	3	1	2	14988.8690	14988.8681	0.0009
3	1	3	2	0	2	15827.1752	15827.1760	-0.0008
6	2	4	6	1	5	16174.0470	16174.0477	-0.0006
5	1	5	4	1	4	16769.7791	16769.7799	-0.0007
4	2	2	4	1	3	17250.4851	17250.4859	-0.0007
5	0	5	4	0	4	17465.5411	17465.5416	-0.0005
5	2	4	4	2	3	17773.0520	17773.0527	-0.0007
3	2	1	3	1	2	17826.0832	17826.0818	0.0014
5	3	3	4	3	2	17869.1435	17869.1433	0.0001
5	3	2	4	3	1	17879.9713	17879.9710	0.0003
5	2	3	4	2	2	18120.3003	18120.2994	0.0009
4	1	4	3	0	3	18650.8515	18650.8526	-0.0010
5	1	4	4	1	3	18698.8854	18698.8847	0.0007

Table S9: *anti*-3-furfural ( $^{13}\text{C}5$ )

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
1	1	0	1	0	1	6562.8672	6562.8674	-0.0002
2	1	2	1	1	1	6683.6798	6683.6786	0.0011
2	1	1	2	0	2	6958.1190	6958.1191	0.0000
2	0	2	1	0	1	7045.2576	7045.2576	0.0000
2	1	1	1	1	0	7440.5094	7440.5092	0.0001
3	1	2	3	0	3	7582.1028	7582.1027	0.0000
4	0	4	3	1	3	8645.6716	8645.6704	0.0012
5	1	4	5	0	5	9664.6529	9664.6535	-0.0005
1	1	1	0	0	0	9715.5017	9715.5013	0.0004
3	1	3	2	1	2	10015.2105	10015.2120	-0.0015
3	0	3	2	0	2	10526.0006	10526.0018	-0.0011
3	2	2	2	2	1	10593.1211	10593.1205	0.0006
3	2	1	2	2	0	10660.2560	10660.2552	0.0007
6	1	5	6	0	6	11207.4873	11207.4866	0.0007
5	0	5	4	1	4	12638.6981	12638.6986	-0.0005
2	1	2	1	0	1	12868.1310	12868.1300	0.0010
7	1	6	7	0	7	13130.9303	13130.9306	-0.0002
4	1	4	3	1	3	13335.0230	13335.0235	-0.0004
4	0	4	3	0	3	13957.7525	13957.7530	-0.0005
4	2	3	3	2	2	14111.0432	14111.0436	-0.0003
4	3	2	3	3	1	14156.4294	14156.4311	-0.0016
4	3	1	3	3	0	14159.2433	14159.2406	0.0026
4	2	2	3	2	1	14277.4460	14277.4461	0.0000
4	1	3	3	1	2	14845.8632	14845.8636	-0.0003



3	1	3	2	0	2	15838.0842	15838.0844	-0.0001
8	2	6	8	1	7	15946.7778	15946.7777	0.0001
7	2	5	7	1	6	16072.0572	16072.0574	-0.0001
6	2	4	6	1	5	16426.9225	16426.9233	-0.0007
6	0	6	5	1	5	16628.8765	16628.8753	0.0012
5	1	5	4	1	4	16640.2475	16640.2480	-0.0004
5	2	3	5	1	4	16934.3196	16934.3188	0.0007
5	0	5	4	0	4	17328.0515	17328.0518	-0.0002
4	2	2	4	1	3	17512.0192	17512.0179	0.0013
5	2	4	4	2	3	17617.7482	17617.7484	-0.0002
5	3	3	4	3	2	17708.2289	17708.2294	-0.0005
5	3	2	4	3	1	17718.0360	17718.0362	-0.0001
5	2	3	4	2	2	17944.7928	17944.7929	0.0000
3	2	1	3	1	2	18080.4353	18080.4353	0.0000
5	1	4	4	1	3	18522.4917	18522.4920	-0.0002
2	2	0	2	1	1	18570.1643	18570.1655	-0.0012
4	1	4	3	0	3	18647.1070	18647.1062	0.0008

Table S10: *anti*-3-furfural ( $^{13}\text{C6}$ )

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
2	1	2	1	1	1	6689.0156	6689.0159	-0.0002
2	1	1	2	0	2	7019.4710	7019.4738	-0.0027
2	0	2	1	0	1	7048.2711	7048.2716	-0.0005
2	1	1	1	1	0	7440.3759	7440.3755	0.0003
3	1	2	3	0	3	7637.9853	7637.9868	-0.0015
4	1	3	4	0	4	8517.5046	8517.5053	-0.0006
4	0	4	3	1	3	8582.6042	8582.6044	-0.0002
5	1	4	5	0	5	9699.4283	9699.4278	0.0005
1	1	1	0	0	0	9784.0400	9784.0403	-0.0003
3	1	3	2	1	2	10023.4652	10023.4663	-0.0010
3	0	3	2	0	2	10531.5395	10531.5402	-0.0006
3	2	2	2	2	1	10597.0226	10597.0224	0.0002
3	2	1	2	2	0	10662.5236	10662.5221	0.0014
3	1	2	2	1	1	11150.0540	11150.0533	0.0007
6	1	5	6	0	6	11225.3469	11225.3474	-0.0004
5	0	5	4	1	4	12578.3905	12578.3903	0.0001
2	1	2	1	0	1	12940.7055	12940.7052	0.0003
4	1	4	3	1	3	13346.4653	13346.4664	-0.0011
4	0	4	3	0	3	13966.9630	13966.9642	-0.0011
4	2	3	3	2	2	14116.5685	14116.5675	0.0010
4	3	1	3	3	0	14163.5584	14163.5569	0.0015
4	2	2	3	2	1	14278.9661	14278.9647	0.0013
4	1	3	3	1	2	14846.4828	14846.4826	0.0002

3	1	3	2	0	2	15915.8994	15915.9000	-0.0005
6	0	6	5	1	5	16573.9906	16573.9906	0.0000
6	2	4	6	1	5	16623.0252	16623.0232	0.0020
5	1	5	4	1	4	16655.1982	16655.1993	-0.0010
5	2	3	5	1	4	17136.7666	17136.7668	-0.0002
5	0	5	4	0	4	17342.2508	17342.2523	-0.0014
5	2	4	4	2	3	17625.1693	17625.1683	0.0010
5	2	3	4	2	2	17944.5264	17944.5251	0.0013
3	2	1	3	1	2	18283.9350	18283.9344	0.0006
5	1	4	4	1	3	18524.1746	18524.1749	-0.0002
4	1	4	3	0	3	18730.8247	18730.8262	-0.0015

Table S11: *anti*-3-furfural (<sup>18</sup>O7)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
2	1	2	1	1	1	6468.3584	6468.3576	0.0008
1	1	0	1	0	1	6681.4130	6681.4122	0.0007
2	0	2	1	0	1	6804.2372	6804.2377	-0.0004
2	1	1	2	0	2	7045.5113	7045.5109	0.0004
2	1	1	1	1	0	7168.3358	7168.3363	-0.0004
3	1	2	3	0	3	7617.7796	7617.7801	-0.0004
4	0	4	3	1	3	7978.7162	7978.7168	-0.0006
4	1	3	4	0	4	8428.1844	8428.1845	-0.0001
5	1	4	5	0	5	9513.1251	9513.1238	0.0012
3	1	3	2	1	2	9693.8825	9693.8818	0.0007
1	1	1	0	0	0	9740.5981	9740.5985	-0.0004
3	0	3	2	0	2	10171.2212	10171.2211	0.0000
3	2	1	2	2	0	10283.7945	10283.7957	-0.0012
3	1	2	2	1	1	10743.4906	10743.4904	0.0002
6	1	5	6	0	6	10910.3961	10910.3965	-0.0004
5	0	5	4	1	4	11839.4800	11839.4807	-0.0007
2	1	2	1	0	1	12799.7793	12799.7797	-0.0003
4	1	4	3	1	3	12909.5116	12909.5115	0.0001
4	0	4	3	0	3	13496.9195	13496.9195	0.0000
4	2	3	3	2	2	13625.6739	13625.6737	0.0001
4	3	2	3	3	1	13663.8089	13663.8096	-0.0007
4	3	1	3	3	0	13665.9434	13665.9431	0.0003
4	2	2	3	2	1	13765.4207	13765.4204	0.0003
4	1	3	3	1	2	14307.3243	14307.3239	0.0003
3	1	3	2	0	2	15689.4240	15689.4239	0.0000
6	0	6	5	1	5	15711.2718	15711.2719	-0.0001
5	1	5	4	1	4	16112.7439	16112.7438	0.0001
5	0	5	4	0	4	16770.2754	16770.2754	0.0000
6	2	4	6	1	5	16921.2929	16921.2924	0.0005

5	2	4	4	2	3	17014.4415	17014.4412	0.0002
5	3	3	4	3	2	17090.6297	17090.6294	0.0002
5	3	2	4	3	1	17098.0798	17098.0801	-0.0003
5	2	3	4	2	2	17289.9243	17289.9245	-0.0002
5	1	4	4	1	3	17855.2151	17855.2147	0.0004
4	2	2	4	1	3	18006.7500	18006.7515	-0.0014
4	1	4	3	0	3	18427.7150	18427.7142	0.0007

Table S12: *syn*-3-furfural (parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
1	1	0	1	0	1	6560.3808	6560.3805	0.0003
2	1	2	1	1	1	6781.7133	6781.7134	-0.0001
3	2	1	4	1	4	6834.8320	6834.8313	0.0007
2	1	1	2	0	2	6967.0812	6967.0809	0.0003
2	0	2	1	0	1	7152.8070	7152.8072	-0.0002
2	2	1	3	1	2	7186.5608	7186.5619	-0.0011
2	1	1	1	1	0	7559.5076	7559.5077	-0.0001
3	1	2	3	0	3	7610.0021	7610.0020	0.0001
4	1	3	4	0	4	8526.4478	8526.4476	0.0002
4	0	4	3	1	3	8888.2179	8888.2180	-0.0001
2	2	0	3	1	3	9537.2368	9537.2371	-0.0003
1	1	1	0	0	0	9756.7908	9756.7908	0.0000
5	1	4	5	0	5	9760.6255	9760.6258	-0.0003
3	1	3	2	1	2	10161.6791	10161.6792	0.0000
5	3	2	6	2	5	10566.4285	10566.4282	0.0002
3	0	3	2	0	2	10684.9355	10684.9353	0.0001
3	2	2	2	2	1	10755.8964	10755.8962	0.0002
3	2	1	2	2	0	10826.8720	10826.8714	0.0005
7	1	6	6	2	5	11021.5922	11021.5924	-0.0001
3	1	2	2	1	1	11327.8564	11327.8564	0.0000
6	1	5	6	0	6	11355.9992	11355.9989	0.0003
5	0	5	4	1	4	12940.0688	12940.0690	-0.0002
2	1	2	1	0	1	12953.1959	12953.1959	0.0000
7	1	6	7	0	7	13344.7521	13344.7521	0.0000
4	3	2	5	2	3	13391.6052	13391.6045	0.0007
4	1	4	3	1	3	13529.2772	13529.2773	0.0000
4	3	1	5	2	4	14005.0323	14005.0315	0.0008
4	0	4	3	0	3	14165.3504	14165.3506	-0.0001
4	2	3	3	2	2	14327.3240	14327.3242	-0.0001
4	3	2	3	3	1	14375.2818	14375.2819	-0.0001
4	3	1	3	3	0	14378.3385	14378.3386	-0.0001
4	2	2	3	2	1	14503.1585	14503.1587	-0.0002
4	1	3	3	1	2	15081.7959	15081.7962	-0.0002

8	1	7	8	0	8	15737.2981	15737.2978	0.0002
8	1	7	7	2	6	15879.0383	15879.0378	0.0004
8	2	6	8	1	7	15929.2716	15929.2712	0.0004
3	1	3	2	0	2	15962.0681	15962.0678	0.0003
7	2	5	7	1	6	16025.2903	16025.2902	0.0000
9	2	7	9	1	8	16145.3876	16145.3873	0.0002
10	2	8	10	1	9	16730.1446	16730.1470	-0.0023
5	1	5	4	1	4	16881.5173	16881.5172	0.0000
6	0	6	5	1	5	16984.5015	16984.5013	0.0002
3	3	1	4	2	2	17248.4567	17248.4581	-0.0013
4	2	2	4	1	3	17452.6022	17452.6016	0.0005
3	3	0	4	2	3	17513.5832	17513.5837	-0.0004
5	0	5	4	0	4	17581.1284	17581.1283	0.0001
11	2	9	11	1	10	17729.7443	17729.7430	0.0012
5	2	4	4	2	3	17886.8908	17886.8908	0.0000
5	3	3	4	3	2	17982.4309	17982.4302	0.0007
5	3	2	4	3	1	17993.0977	17993.0979	-0.0001
3	2	1	3	1	2	18031.2396	18031.2391	0.0004
5	2	3	4	2	2	18232.1351	18232.1355	-0.0004
9	1	8	9	0	9	18515.8353	18515.8357	-0.0003
2	2	0	2	1	1	18532.2235	18532.2241	-0.0005
4	1	4	3	0	3	18806.4100	18806.4098	0.0002
5	1	4	4	1	3	18815.3065	18815.3066	0.0000

Table S13: *syn*-3-furfural (<sup>13</sup>C2)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
2	1	2	1	1	1	6764.8049	6764.8049	0.0000
2	0	2	1	0	1	7139.7819	7139.7830	-0.0011
3	1	2	3	0	3	7503.6091	7503.6099	-0.0008
2	1	1	1	1	0	7551.9511	7551.9507	0.0004
3	1	3	2	1	2	10135.8391	10135.8400	-0.0008
3	0	3	2	0	2	10663.4479	10663.4475	0.0004
3	2	2	2	2	1	10737.5462	10737.5461	0.0001
3	1	2	2	1	1	11316.0055	11316.0052	0.0003
2	1	2	1	0	1	12810.1176	12810.1158	0.0018
5	0	5	4	1	4	13032.3852	13032.3847	0.0004
4	1	4	3	1	3	13493.9899	13493.9902	-0.0002
4	0	4	3	0	3	14133.2131	14133.2139	-0.0007
4	2	3	3	2	2	14302.2412	14302.2409	0.0002
4	2	2	3	2	1	14485.7469	14485.7460	0.0008
4	1	3	3	1	2	15064.9752	15064.9755	-0.0002
3	1	3	2	0	2	15806.1727	15806.1728	0.0000
5	1	5	4	1	4	16836.1781	16836.1783	-0.0002

6	0	6	5	1	5	17061.7030	17061.7024	0.0005
5	0	5	4	0	4	17535.8857	17535.8863	-0.0005
5	2	4	4	2	3	17854.5495	17854.5492	0.0002
5	2	3	4	2	2	18214.4437	18214.4441	-0.0003
5	1	4	4	1	3	18792.5197	18792.5203	-0.0005

Table S14: *syn*-3-furfural ( $^{13}\text{C}3$ )

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
2	1	2	1	1	1	6779.5380	6779.5381	-0.0002
2	1	1	2	0	2	6960.7150	6960.7157	-0.0003
2	0	2	1	0	1	7150.7050	7150.7051	0.0003
2	1	1	1	1	0	7557.5340	7557.5339	0.0003
3	1	2	3	0	3	7603.8790	7603.8791	-0.0005
4	1	3	4	0	4	8520.7330	8520.7330	-0.0003
4	0	4	3	1	3	8890.5280	8890.5289	-0.0007
3	1	3	2	1	2	10158.4000	10158.3998	0.0000
3	0	3	2	0	2	10681.7100	10681.7144	0.0002
3	2	2	2	2	1	10752.7800	10752.7848	-0.0002
3	2	1	2	2	0	10823.8700	10823.8690	-0.0014
3	1	2	2	1	1	11324.8800	11324.8778	0.0003
6	1	5	6	0	6	11351.7700	11351.7662	0.0008
5	0	5	4	1	4	12941.0900	12941.0878	0.0009
2	1	2	1	0	1	12944.4300	12944.4264	0.0003
7	1	6	7	0	7	13341.5800	13341.5770	-0.0004
4	1	4	3	1	3	13524.8800	13524.8761	-0.0005
4	0	4	3	0	3	14160.9400	14160.9355	-0.0003
4	2	3	3	2	2	14323.1500	14323.1543	0.0003
4	2	2	3	2	1	14499.2600	14499.2551	0.0019
4	1	3	3	1	2	15077.7900	15077.7894	-0.0009
3	1	3	2	0	2	15952.1200	15952.1210	0.0006
5	1	5	4	1	4	16875.9700	16875.9738	-0.0001
5	0	5	4	0	4	17575.4300	17575.4351	-0.0001
5	2	4	4	2	3	17881.6400	17881.6445	-0.0003
5	2	3	4	2	2	18227.4000	18227.3962	0.0000
4	1	4	3	0	3	18795.2800	18795.2827	0.0000
5	1	4	4	1	3	18810.2400	18810.2366	0.0000

Table S15: *syn*-3-furfural ( $^{13}\text{C}4$ )

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
2	1	2	1	1	1	6745.9462	6745.9455	0.0007
2	1	1	2	0	2	6801.2756	6801.2776	-0.0020
2	0	2	1	0	1	7121.4105	7121.4102	0.0002

3	1	2	3	0	3	7455.6251	7455.6259	-0.0008
2	1	1	1	1	0	7534.5069	7534.5061	0.0008
4	1	3	4	0	4	8390.4514	8390.4515	-0.0001
3	1	3	2	1	2	10107.4185	10107.4191	-0.0006
3	0	3	2	0	2	10635.3471	10635.3463	0.0007
3	2	1	2	2	0	10785.3049	10785.3072	-0.0022
3	1	2	2	1	1	11289.6964	11289.6946	0.0018
2	1	2	1	0	1	12739.8469	12739.8462	0.0006
5	0	5	4	1	4	13034.8798	13034.8791	0.0006
4	1	4	3	1	3	13455.8660	13455.8662	-0.0002
4	0	4	3	0	3	14094.7844	14094.7835	0.0008
4	2	3	3	2	2	14265.7685	14265.7681	0.0003
4	2	2	3	2	1	14451.3997	14451.4002	-0.0005
4	1	3	3	1	2	15029.6105	15029.6091	0.0014
3	1	3	2	0	2	15725.8533	15725.8551	-0.0017
5	1	5	4	1	4	16788.1883	16788.1883	0.0000
4	2	2	4	1	3	16917.8953	16917.8946	0.0007
6	0	6	5	1	5	17051.2670	17051.2663	0.0007
5	0	5	4	0	4	17486.4707	17486.4706	0.0000
3	2	1	3	1	2	17496.1047	17496.1035	0.0012
5	2	4	4	2	3	17808.6835	17808.6847	-0.0012
5	2	3	4	2	2	18172.6138	18172.6147	-0.0008
4	1	4	3	0	3	18546.3744	18546.3750	-0.0006
5	1	4	4	1	3	18747.8161	18747.8163	-0.0002

Table S16: *syn*-3-furfural ( $^{13}\text{C}5$ )

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
2	1	1	2	0	2	6948.6139	6948.6145	-0.0005
2	0	2	1	0	1	7056.0648	7056.0642	0.0006
3	1	2	3	0	3	7575.1808	7575.1799	0.0009
4	1	3	4	0	4	8467.2228	8467.2217	0.0010
4	0	4	3	1	3	8681.2811	8681.2824	-0.0013
5	1	4	5	0	5	9667.2527	9667.2541	-0.0014
3	1	3	2	1	2	10029.4918	10029.4912	0.0005
3	0	3	2	0	2	10541.8316	10541.8307	0.0009
3	2	2	2	2	1	10609.5643	10609.5633	0.0010
3	1	2	2	1	1	11168.3963	11168.3960	0.0002
6	1	5	6	0	6	11217.5424	11217.5419	0.0005
5	0	5	4	1	4	12679.9460	12679.9451	0.0008
2	1	2	1	0	1	12865.2931	12865.2936	-0.0005
7	1	6	7	0	7	13150.2568	13150.2566	0.0001
4	1	4	3	1	3	13353.8990	13353.8980	0.0009
4	0	4	3	0	3	13978.1737	13978.1724	0.0013

4	2	3	3	2	2	14132.8463	14132.8470	-0.0006
4	2	2	3	2	1	14300.7499	14300.7512	-0.0012
4	1	3	3	1	2	14870.2131	14870.2143	-0.0012
3	1	3	2	0	2	15838.7208	15838.7207	0.0000
5	1	5	4	1	4	16663.5960	16663.5963	-0.0003
6	0	6	5	1	5	16674.9080	16674.9070	0.0009
5	0	5	4	0	4	17352.5608	17352.5608	0.0000
5	2	4	4	2	3	17644.8095	17644.8100	-0.0005
5	2	3	4	2	2	17974.7446	17974.7451	-0.0005
5	1	4	4	1	3	18552.5924	18552.5931	-0.0007

Table S17: *syn*-3-furfural (<sup>13</sup>C6)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{obs}/\text{MHz}$	$\nu_{calc}/\text{MHz}$	$\nu_{obs-calc}/\text{MHz}$
2	1	2	1	1	1	6711.5272	6711.5278	-0.0005
2	0	2	1	0	1	7076.4726	7076.4719	0.0007
2	1	1	1	1	0	7475.8753	7475.8744	0.0008
3	1	2	3	0	3	7574.1364	7574.1380	-0.0015
4	1	3	4	0	4	8472.7522	8472.7514	0.0007
4	0	4	3	1	3	8735.5526	8735.5534	-0.0007
3	1	3	2	1	2	10056.7481	10056.7487	-0.0005
3	0	3	2	0	2	10571.8526	10571.8532	-0.0006
3	1	2	2	1	1	11202.7797	11202.7785	0.0012
6	1	5	6	0	6	11244.6416	11244.6430	-0.0013
5	0	5	4	1	4	12745.2617	12745.2620	-0.0002
2	1	2	1	0	1	12873.1656	12873.1640	0.0015
4	1	4	3	1	3	13389.9853	13389.9868	-0.0015
4	0	4	3	0	3	14017.1402	14017.1409	-0.0007
4	2	3	3	2	2	14173.9548	14173.9546	0.0001
4	2	2	3	2	1	14344.1826	14344.1818	0.0008
4	1	3	3	1	2	14915.7550	14915.7544	0.0006
3	1	3	2	0	2	15853.4419	15853.4408	0.0011
5	1	5	4	1	4	16708.3251	16708.3276	-0.0024
6	0	6	5	1	5	16750.0613	16750.0596	0.0016
5	0	5	4	0	4	17399.6931	17399.6954	-0.0022
5	2	4	4	2	3	17695.8973	17695.8970	0.0002
5	3	3	4	3	2	17788.4297	17788.4301	-0.0003
5	2	3	4	2	2	18030.3116	18030.3096	0.0019
5	1	4	4	1	3	18608.9995	18608.9990	0.0005

#### Appendix IV: Kraitchman Coordinates ( $r_s$ )

Table S18:  $r_s$  coordinates for *anti*-3-furfural

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<sup>18</sup>O1

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	a	b	
PLANAR:	1.93665 +- 0.00000	0.47092 +- 0.00000	
+Costain err.	1.93665 +- 0.00077	0.47092 +- 0.00319	
	a	b	c
NONPLANAR:	1.93659 +- 0.00000	0.47064 +- 0.00001	0.01620 +- 0.00021
+Costain err.	1.93659 +- 0.00077	0.47064 +- 0.00319	0.01620 +- 0.09260

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<sup>13</sup>C2

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	a	b	
PLANAR:	0.73211 +- 0.00001	1.09721 +- 0.00000	
+Costain err.	0.73211 +- 0.00205	1.09721 +- 0.00137	
	a	b	c
NONPLANAR:	0.73273 +- 0.00001	1.09764 +- 0.00001	0.03054*i+- 0.00023
+Costain err.	0.73273 +- 0.00205	1.09764 +- 0.00137	0.03054*i+- 0.04912

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<sup>13</sup>C3

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	a	b	
PLANAR:	0.25466 +- 0.00002	0.18201 +- 0.00001	
+Costain err.	0.25466 +- 0.00589	0.18201 +- 0.00824	
	a	b	c
NONPLANAR:	0.25350 +- 0.00002	0.18037 +- 0.00003	0.02437 +- 0.00020
+Costain err.	0.25350 +- 0.00592	0.18037 +- 0.00832	0.02437 +- 0.06155

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<sup>13</sup>C4

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	a	b	
PLANAR:	0.33110 +- 0.00004	1.10995 +- 0.00000	
+Costain err.	0.33110 +- 0.00453	1.10995 +- 0.00135	
	a	b	c
NONPLANAR:	0.33180 +- 0.00003	1.11017 +- 0.00001	0.02196*i+- 0.00052
+Costain err.	0.33180 +- 0.00452	1.11017 +- 0.00135	0.02196*i+- 0.06831

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<sup>13</sup>C5

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	a	b	
PLANAR:	1.67610 +- 0.00000	0.87545 +- 0.00000	
+Costain err.	1.67610 +- 0.00089	0.87545 +- 0.00171	
	a	b	c
NONPLANAR:	1.67621 +- 0.00000	0.87567 +- 0.00001	0.01958*i+- 0.00038
+Costain err.	1.67621 +- 0.00089	0.87567 +- 0.00171	0.01958*i+- 0.07660

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<sup>13</sup>C6  
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	a	b	
PLANAR:	1.70649 +- 0.00001	0.50230 +- 0.00000	
+Costain err.	1.70649 +- 0.00088	0.50230 +- 0.00299	
	a	b	c
NONPLANAR:	1.70637 +- 0.00000	0.50189 +- 0.00001	0.02027 +- 0.00035
+Costain err.	1.70637 +- 0.00088	0.50189 +- 0.00299	0.02027 +- 0.07401

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<sup>18</sup>O7  
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	a	b	
PLANAR:	2.58544 +- 0.00000	0.33559 +- 0.00000	
+Costain err.	2.58544 +- 0.00058	0.33559 +- 0.00447	
	a	b	c
NONPLANAR:	2.58545 +- 0.00000	0.33571 +- 0.00001	0.00909*i+- 0.00027
+Costain err.	2.58545 +- 0.00058	0.33571 +- 0.00447	0.00909*i+- 0.16508

Table S18: r<sub>s</sub> coordinates for *syn*-3-furfural

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<sup>13</sup>C2  
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	a	b	
PLANAR:	0.30398 +- 0.00003	0.99300 +- 0.00000	
+Costain err.	0.30398 +- 0.00493	0.99300 +- 0.00151	
	a	b	c
NONPLANAR:	0.30429 +- 0.00002	0.99310 +- 0.00001	0.01390*i+- 0.00051
+Costain err.	0.30429 +- 0.00493	0.99310 +- 0.00151	0.01390*i+- 0.10794

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<sup>13</sup>C3  
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	a	b	
PLANAR:	0.24568 +- 0.00002	0.23252 +- 0.00001	
+Costain err.	0.24568 +- 0.00611	0.23252 +- 0.00645	
	a	b	c
NONPLANAR:	0.24466 +- 0.00002	0.23144 +- 0.00002	0.02235 +- 0.00022
+Costain err.	0.24466 +- 0.00613	0.23144 +- 0.00648	0.02235 +- 0.06711

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<sup>13</sup>C4  
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	a	b	
PLANAR:	0.79316 +- 0.00001	1.19663 +- 0.00000	
+Costain err.	0.79316 +- 0.00189	1.19663 +- 0.00125	
	a	b	c
NONPLANAR:	0.79383 +- 0.00001	1.19710 +- 0.00001	0.03336*i+- 0.00024
+Costain err.	0.79383 +- 0.00189	1.19710 +- 0.00125	0.03336*i+- 0.04497

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<sup>13</sup>C5  
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	a	b	
PLANAR:	1.94451 +- 0.00000	0.47126 +- 0.00000	
+Costain err.	1.94451 +- 0.00077	0.47126 +- 0.00318	
	a	b	c
NONPLANAR:	1.94442 +- 0.00000	0.47087 +- 0.00001	0.01911 +- 0.00032
+Costain err.	1.94442 +- 0.00077	0.47087 +- 0.00319	0.01911 +- 0.07851

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<sup>13</sup>C6  
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	a	b	
PLANAR:	1.71504 +- 0.00001	0.50278 +- 0.00001	
+Costain err.	1.71504 +- 0.00087	0.50278 +- 0.00298	
	a	b	c
NONPLANAR:	1.71487 +- 0.00001	0.50221 +- 0.00002	0.02394 +- 0.00041
+Costain err.	1.71487 +- 0.00087	0.50221 +- 0.00299	0.02394 +- 0.06265