

Electronic Supporting Information

Communication through the Furan Ring: Conformational Effect on the Internal Rotation of 5-Methylfurfural Studied by Microwave Spectroscopy

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Quantum Chemical Data

Table S-1. Cartesian coordinates of the *trans* conformer of 5-methylfurfural in the principal axis of inertia as optimized at the MP2/6-311++G(d,p) level of theory.

Atom	a / Å	b / Å	c / Å
C	1.440099	-0.181338	0.000017
C	1.424018	1.197301	0.000000
C	0.055784	1.582753	-0.000017
C	-0.672084	0.407157	0.000008
O	0.168187	-0.661569	-0.000059
H	2.295073	1.837283	0.000011
H	-0.357597	2.582395	-0.000024
C	2.532767	-1.190452	0.000025
H	2.472060	-1.829310	0.886138
H	2.472107	-1.829269	-0.886123
H	3.499051	-0.681885	0.000062
C	-2.113341	0.181908	0.000030
O	-2.653152	-0.912613	0.000000
H	-2.700892	1.122341	0.000117

Table S-2. Cartesian coordinates of the *cis* conformer of 5-methylfurfural in the principal axis of inertia as optimized at the MP2/6-311++G(d,p) level of theory.

Atom	a / Å	b / Å	c / Å
C	-1.545804	-0.025740	-0.000242
C	-1.159819	1.298609	-0.000041
C	0.260832	1.312581	0.000176
C	0.653503	-0.010895	0.000592
O	-0.445256	-0.823623	0.000031
H	-1.830369	2.146617	-0.000378
H	0.930427	2.161017	0.000330
C	-2.869185	-0.705135	-0.000151
H	-2.985216	-1.336387	-0.886425
H	-2.985649	-1.335275	0.886860
H	-3.662456	0.045322	-0.000808
H	1.955740	-0.671960	0.000357
O	3.017747	-0.068640	-0.000559
H	1.910750	-1.778383	0.000562

Microwave Spectroscopic Data

Table S-3a. Observed frequencies (*Obs.*) of the A species transitions of the *trans* conformer of 5-methylfurfural included in the XIAM fit.

<i>Upper Level</i>			<i>Lower Level</i>			<i>Obs.</i> ^[a]	<i>Obs.-calc.</i> ^[b]
<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>GHz</i>	<i>kHz</i>
1	0	1	0	0	0	2.6457366	-1.1
1	1	1	0	0	0	5.9037757	0.2
1	1	0	1	0	1	3.6087955	3.1
2	0	2	1	0	1	5.2646488	-1.4
2	1	2	1	0	1	8.1987587	-0.9
2	1	1	1	1	0	5.6422270	-1.9
2	2	1	1	1	0	15.4163098	0.0
2	1	2	1	1	1	4.9407196	-2.2
2	2	0	1	1	1	15.7938875	1.1
2	1	1	2	0	2	3.9863746	3.4
3	0	3	2	0	2	7.8309418	0.7
3	1	3	2	0	2	10.3290183	-1.2
2	2	0	2	1	1	9.8009029	0.1
3	1	2	2	1	1	8.4458792	-0.1
3	2	2	2	1	1	17.7112999	-0.4
2	2	1	2	1	2	10.8263465	3.9
3	0	3	2	1	2	4.8968327	1.0
3	1	3	2	1	2	7.3949093	-0.8
3	2	1	2	1	2	18.8966436	0.1
3	2	1	2	2	0	8.0434783	-0.6
3	2	2	2	2	1	7.9372181	-1.4
4	0	4	3	0	3	10.3236544	-1.2
4	1	4	3	0	3	12.3295127	0.0
3	2	1	3	1	2	9.3985034	1.0
4	1	3	3	1	2	11.2267438	0.5
4	2	3	3	1	2	19.8274744	-0.4
3	2	2	3	1	3	11.3686497	-2.3
4	0	4	3	1	3	7.8255769	-0.4
4	1	4	3	1	3	9.8314344	0.1
3	3	0	3	2	1	17.0512715	-0.2
4	2	2	3	2	1	10.8212668	0.2
4	3	2	3	2	1	27.6829598	5.7
3	3	1	3	2	2	17.1830665	-0.3
4	2	3	3	2	2	10.5620536	-0.3
4	3	1	3	2	2	27.8250099	-1.1
4	3	2	3	3	1	10.6329695	0.7
4	1	3	4	0	4	5.5043999	2.9
5	0	5	4	0	4	12.7338533	-0.3
5	1	5	4	0	4	14.2529908	1.1
4	2	2	4	1	3	8.9930256	0.0
5	1	4	4	1	3	13.9741692	-0.4
4	2	3	4	1	4	12.0992766	5.1
5	0	5	4	1	4	10.7279963	-0.2
5	1	5	4	1	4	12.2471311	-1.5
4	3	1	4	2	2	16.8706618	-1.1
5	2	3	4	2	2	13.6634497	-1.2
5	3	3	4	2	2	30.1698079	-2.5
4	3	2	4	2	3	17.2539819	0.2
5	1	4	4	2	3	5.3734377	-0.4

5	2	4	4	2	3	13.1690861	-0.5
5	3	2	4	2	3	30.5977728	-0.6
5	3	2	4	3	1	13.3348155	-0.8
5	3	3	4	3	2	13.3081230	0.0
6	0	6	5	0	5	15.0704507	-0.8
6	1	6	5	0	5	16.1599073	-1.6
5	2	3	5	1	4	8.6823069	0.0
6	1	5	5	1	4	16.6750921	0.6
5	2	4	5	1	5	13.0212246	-0.8
6	2	4	5	1	5	30.4640782	-1.9
5	3	2	5	2	3	16.5420283	0.0
6	3	4	5	2	3	32.4948615	-1.6
6	1	5	5	2	4	8.8794430	0.1
6	2	5	5	2	4	15.7541578	-1.7
6	3	3	5	2	4	33.4873078	-1.6
6	3	3	5	3	2	16.0586234	0.9
6	3	4	5	3	3	15.9885034	-0.2
6	1	5	6	0	6	8.3493538	0.8
7	1	7	6	0	6	18.1024426	-2.2
6	2	4	6	1	5	8.5634105	-1.2
7	1	6	6	1	5	19.3142666	-0.9
7	1	7	6	1	6	17.0129869	-0.6
7	2	5	6	1	6	35.2936353	4.2
6	3	3	6	2	4	16.0444539	-0.8
7	2	5	6	2	4	19.4703234	-0.4
6	3	4	6	2	5	17.6273620	-0.2
7	1	6	6	2	5	12.4395503	-0.7
7	2	6	6	2	5	18.3135212	-1.4
7	3	4	6	3	3	18.8239025	0.1
7	3	5	6	3	4	18.6701156	0.0
7	1	6	7	0	7	10.3064812	-2.8
7	2	5	7	1	6	8.7194673	-0.7
7	2	6	7	1	7	15.4351496	2.3
8	0	8	7	1	7	18.8752350	-4.9
8	1	8	7	1	7	19.3659072	-1.1
7	3	4	7	2	5	15.3980327	-0.6
7	3	5	7	2	6	17.9839545	-0.6
8	2	6	7	3	5	7.2342701	-0.7
8	2	6	8	1	7	9.2161098	0.7
9	2	8	8	1	7	28.1857162	-5.1
9	2	7	8	3	6	11.1231126	-1.8
9	2	7	9	1	8	10.1036041	0.8
10	2	9	9	1	8	29.6484688	-3.6
9	3	6	9	2	7	13.9550327	0.8

^[a] Observed frequencies in GHz.

^[b] Observed – calculated frequencies in kHz as obtained after a fit with the program *XIAM*.

Table S-3b. Observed frequencies (*Obs.*) of the E species transitions of the *trans* conformer of 5-methylfurfural included in the XIAM fit.

<i>Upper Level</i>			<i>Lower Level</i>			<i>Obs.</i> ^[a]	<i>Obs.-calc.</i> ^[b]
<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>J</i>	<i>K_a</i>	<i>K_c</i>		
1	0	1	0	0	0	2.6456807	0.4
1	1	1	0	0	0	5.9024481	0.4
1	1	0	1	0	1	3.6088756	0.2
2	0	2	1	0	1	5.2645408	-0.1
2	1	2	1	0	1	8.1979025	0.3
2	1	1	1	1	0	5.6416136	0.0
2	1	2	1	1	1	4.9411356	0.9
2	2	0	1	1	1	15.8132823	-11.1
2	1	1	2	0	2	3.9859480	0.0
3	0	3	2	0	2	7.8307901	0.4
3	1	3	2	0	2	10.3283108	0.6
2	2	0	2	1	1	9.8195653	-6.5
3	1	2	2	1	1	8.4455365	0.8
3	2	2	2	1	1	17.7022355	0.3
2	2	1	2	1	2	10.8040576	3.1
3	0	3	2	1	2	4.8974287	0.3
3	1	3	2	1	2	7.3949495	0.5
3	2	1	2	1	2	18.9017724	1.8
3	2	1	2	2	0	8.0296091	-2.9
3	2	2	2	2	1	7.9507633	-4.3
4	0	4	3	0	3	10.3234744	0.7
4	1	4	3	0	3	12.3289028	1.2
3	2	1	3	1	2	9.4036485	0.4
4	1	3	3	1	2	11.2263914	0.4
4	2	3	3	1	2	19.8230734	0.9
3	2	2	3	1	3	11.3598719	-1.2
4	0	4	3	1	3	7.8259538	0.6
4	1	4	3	1	3	9.8313821	1.0
3	3	0	3	2	1	17.0875933	2.3
4	2	2	3	2	1	10.8165143	0.3
4	3	2	3	2	1	27.7243309	6.6
3	3	1	3	2	2	17.1407455	-1.4
4	2	3	3	2	2	10.5663748	1.9
4	1	3	4	0	4	5.5036114	-0.1
5	0	5	4	0	4	12.7336535	0.5
5	1	5	4	0	4	14.2524665	1.5
4	2	2	4	1	3	8.9937719	0.8
5	1	4	4	1	3	13.9737648	0.5
4	2	3	4	1	4	12.0948652	0.2
5	0	5	4	1	4	10.7282259	0.8
5	1	5	4	1	4	12.2470379	0.9
4	3	1	4	2	2	16.9078113	0.9
5	2	3	4	2	2	13.6617719	1.7
4	3	2	4	2	3	17.2108444	-1.2
5	1	4	4	2	3	5.3770836	0.7
5	2	4	4	2	3	13.1702146	2.3
5	3	2	4	3	1	13.3241360	0.5
5	3	3	4	3	2	13.3182710	0.1
6	0	6	5	0	5	15.0702445	1.7
6	1	6	5	0	5	16.1594645	1.2
5	2	3	5	1	4	8.6817770	0.0

6	1	5	5	1	4	16.6746212	-5.5
5	2	4	5	1	5	13.0180401	-0.1
6	2	4	5	1	5	30.4619768	-0.2
5	3	2	5	2	3	16.5701788	3.2
6	1	5	5	2	4	8.8814978	0.4
6	2	5	5	2	4	15.7543850	1.9
6	3	3	5	2	4	33.5024711	-7.0
6	3	3	5	3	2	16.0436558	1.0
6	3	4	5	3	3	16.0028249	1.4
6	1	5	6	0	6	8.3481062	-0.5
7	1	7	6	0	6	18.1020709	2.0
6	2	4	6	1	5	8.5624387	-0.7
7	1	6	6	1	5	19.3137494	0.2
7	1	7	6	1	6	17.0128488	0.5
7	2	5	6	1	6	35.2909390	0.3
6	3	3	6	2	4	16.0585428	1.5
7	2	5	6	2	4	19.4696144	1.2
6	3	4	6	2	5	17.6073429	-1.7
7	1	6	6	2	5	12.4408633	-0.2
7	2	6	6	2	5	18.3134168	1.5
7	3	4	6	3	3	18.8139528	0.9
7	3	5	6	3	4	18.6793009	2.6
7	1	6	7	0	7	10.3049262	-2.3
7	2	5	7	1	6	8.7183036	0.2
7	2	6	7	1	7	15.4323391	0.2
8	0	8	7	1	7	18.8752060	4.2
8	1	8	7	1	7	19.3657590	2.2
7	3	4	7	2	5	15.4028829	2.8
7	3	5	7	2	6	17.9732270	-0.6
8	2	6	7	3	5	7.2445617	1.2
8	2	6	8	1	7	9.2148119	-0.5
9	2	8	8	1	7	28.1842578	4.1
9	2	7	8	3	6	11.1288781	2.9
9	2	7	9	1	8	10.1021570	-1.1
10	2	9	9	1	8	29.6471943	2.3
9	3	6	9	2	7	13.9542634	1.6

^[a] Observed frequencies in GHz.

^[b] Observed – calculated frequencies in kHz as obtained after a fit with the program *XIAM*.

Table S-4a. Observed frequencies (*Obs.*) of the A species transitions of the *cis* conformer of 5-methylfurfural included in the XIAM fit.

<i>Upper Level</i>			<i>Lower Level</i>			<i>Obs.</i> ^[a]	<i>Obs.-calc.</i> ^[b]
<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>J</i>	<i>K_a</i>	<i>K_c</i>		
2	0	2	1	0	1	4.8137499	-0.9
2	1	1	1	1	0	5.0400689	-2.1
2	1	2	1	1	1	4.6015551	-1.9
3	0	3	2	0	2	7.2030125	-0.1
3	1	2	2	1	1	7.5556161	0.7
3	1	3	2	1	2	6.8979854	-2.3
3	2	1	2	2	0	7.2594207	-1.6
3	2	2	2	2	1	7.2312096	-5.1
4	0	4	3	0	3	9.5714198	-0.6
4	1	3	3	1	2	10.0655705	1.0
4	1	4	3	1	3	9.1893974	-0.3
4	2	2	3	2	1	9.7063201	0.5
4	2	3	3	2	2	9.6361193	-0.4
4	3	1	3	3	0	9.6561691	-1.2
4	3	2	3	3	1	9.6553258	8.9
5	0	5	4	0	4	11.9129099	0.6
5	1	4	4	1	3	12.5677326	1.5
5	1	5	4	1	4	11.4744351	0.1
5	2	3	4	2	2	12.1754098	0.3
5	2	4	4	2	3	12.0363163	0.2
5	3	2	4	3	1	12.0778008	-2.4
6	0	6	5	0	5	14.2228932	-1.5
6	1	5	5	1	4	15.0596047	0.5
6	1	6	5	1	5	13.7520052	-2.2
6	2	4	5	2	3	14.6700782	1.9
6	2	5	5	2	4	14.4306410	0.5
6	3	3	5	3	2	14.5052967	-0.7
6	3	4	5	3	3	14.4973647	0.9
7	0	7	6	0	6	16.4992142	-2.3
7	1	6	6	1	5	17.5383303	1.6
7	1	7	6	1	6	16.0213237	-1.3
7	2	5	6	2	4	17.1912562	2.8
7	2	6	6	2	5	16.8179497	0.4
7	3	4	6	3	3	16.9406254	-0.5
7	3	5	6	3	4	16.9228505	-0.5
8	2	6	7	2	5	19.7366642	1.4
8	2	7	7	2	6	19.1971344	0.8
8	3	6	7	3	5	19.3508596	0.9
12	1	11	11	1	10	29.6075182	-3.2
13	1	13	12	1	12	29.4593768	-3.8
14	1	13	13	1	12	34.2132267	-1.4
15	1	14	14	1	13	36.4606545	-2.1
15	1	15	14	1	14	33.8835415	-6.2

^[a] Observed frequencies in GHz.

^[b] Observed – calculated frequencies in kHz as obtained after a fit with the program *XIAM*.

Table S4-b. Observed frequencies (*Obs.*) of the E species transitions of the *cis* conformer of 5-methylfurfural included in the XIAM fit.

<i>Upper Level</i>			<i>Lower Level</i>			<i>Obs.</i> ^[a]	<i>Obs.-calc.</i> ^[b]
<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>J</i>	<i>K_a</i>	<i>K_c</i>		
2	0	2	1	0	1	4.8137135	0.7
2	1	1	1	1	0	5.0381735	-0.6
2	1	2	1	1	1	4.6033866	0.2
3	0	3	2	0	2	7.2029539	0.6
3	1	2	2	1	1	7.5550692	-0.7
3	1	3	2	1	2	6.8984303	0.5
3	2	1	2	2	0	7.2481462	-4.9
3	2	2	2	2	1	7.2423846	-3.7
4	0	4	3	0	3	9.5713379	0.5
4	1	3	3	1	2	10.0652770	-0.2
4	1	4	3	1	3	9.1895493	0.5
4	2	2	3	2	1	9.6908697	0.3
4	2	3	3	2	2	9.6514432	0.1
4	3	1	3	3	0	9.6556529	-1.0
4	3	2	3	3	1	9.6557013	-1.7
5	0	5	4	0	4	11.9127995	0.4
5	1	4	4	1	3	12.5675030	0.2
5	1	5	4	1	4	11.4744823	1.0
5	2	3	4	2	2	12.1653455	3.5
5	2	4	4	2	3	12.0462310	1.1
5	3	2	4	3	1	12.0762104	-1.3
6	0	6	5	0	5	14.2227551	0.7
6	1	5	5	1	4	15.0593835	-0.4
6	1	6	5	1	5	13.7520034	1.7
6	2	4	5	2	3	14.6653575	-1.0
6	2	5	5	2	4	14.4351803	1.1
6	3	3	5	3	2	14.5013748	-2.0
6	3	4	5	3	3	14.5010939	-0.9
7	0	7	6	0	6	16.4990452	0.6
7	1	6	6	1	5	17.5380926	-0.9
7	1	7	6	1	6	16.0212888	1.9
7	2	5	6	2	4	17.1890090	-0.4
7	2	6	6	2	5	16.8199897	1.3
7	3	4	6	3	3	16.9327591	-0.8
7	3	5	6	3	4	16.9304987	-1.3
8	2	6	7	2	5	19.7354802	-1.1
8	2	7	7	2	6	19.1980822	1.7
8	3	6	7	3	5	19.3631760	0.7
12	1	11	11	1	10	29.6070714	-2.6
12	1	12	11	1	11	27.2387549	3.2
13	0	13	12	0	12	29.6696296	1.9
13	0	13	12	0	12	29.6696287	1.0
13	1	13	12	1	12	29.4592402	1.0
14	0	14	13	0	13	31.8387817	0.2
14	1	13	13	1	12	34.2126574	1.1
15	1	14	14	1	13	36.4600281	5.2
15	1	15	14	1	14	33.8833894	3.7

^[a] Observed frequencies in GHz.

^[b] Observed – calculated frequencies in kHz as obtained after a fit with the program *XIAM*.