

Broadband Microwave Spectroscopy of 2-Furanyloxy Radical: Primary Pyrolysis Product of the Second-Generation Biofuel 2-Methoxyfuran

Supplementary Data

Table S1. Rotational transitions assigned to the 2-furanyloxy radical

J'	k'_a	k'_c	F'	J''	k''_a	k''_c	F''	obs	obs-calc
2	1	1	5/2	2	1	2	5/2	3740.8436	0.0274
5	2	3	11/2	5	2	4	11/2	5931.5011	0.0245
5	2	3	9/2	5	2	4	9/2	5950.6467	0.0388
1	1	0	3/2	1	0	1	3/2	6117.4883	0.0381
1	1	0	1/2	1	0	1	1/2	6147.2248	0.0131
1	0	1	3/2	0	0	0	1/2	6786.8924	0.0173
1	0	1	1/2	0	0	0	1/2	6797.0097	0.0303
3	1	2	7/2	3	1	3	7/2	7463.1598	-0.0322
3	1	2	5/2	3	1	3	5/2	7491.1279	0.0484
2	1	1	5/2	2	0	2	5/2	7577.8591	0.0349
2	1	1	3/2	2	0	2	3/2	7602.8436	-0.0104
2	0	2	3/2	1	1	1	1/2	8568.7760	0.0536
2	0	2	5/2	1	1	1	3/2	8575.1495	0.0417
3	1	2	7/2	3	0	3	7/2	10111.6903	0.0603
3	1	2	5/2	3	0	3	5/2	10139.8796	0.0194
3	1	2	5/2	3	0	3	7/2	10157.7355	0.0231
6	2	4	13/2	6	2	5	13/2	10348.1265	0.0325
6	2	4	11/2	6	2	5	11/2	10374.7743	-0.0188
1	1	1	3/2	0	0	0	1/2	11658.7675	0.0218
1	1	1	1/2	0	0	0	1/2	11686.5674	0.0365
4	1	3	9/2	4	1	4	7/2	12307.5965	0.0240
2	1	2	3/2	1	1	1	1/2	12324.3650	0.0326
4	1	3	9/2	4	1	4	9/2	12324.9117	-0.0684
2	1	2	5/2	1	1	1	3/2	12332.1653	-0.0221
2	1	2	3/2	1	1	1	3/2	12352.1648	0.0513
4	1	3	7/2	4	1	4	7/2	12360.1613	0.0557
4	1	3	7/2	4	1	4	9/2	12377.4750	0.0644
2	0	2	5/2	1	0	1	3/2	13426.6339	-0.0272
2	0	2	3/2	1	0	1	1/2	13429.9196	0.0721
2	0	2	3/2	1	0	1	3/2	13439.6339	0.0109
4	2	2	9/2	4	1	3	9/2	13566.3093	0.0203
4	2	2	7/2	4	1	3	7/2	13583.7067	0.0329
3	2	1	7/2	3	1	2	5/2	13866.1985	0.0526
3	2	1	7/2	3	1	2	7/2	13912.2438	-0.0194
3	2	1	5/2	3	1	2	5/2	13932.4703	0.0147
4	1	3	9/2	4	0	4	9/2	13936.6281	-0.0658
4	1	3	7/2	4	0	4	7/2	13970.7166	0.0305
3	2	1	5/2	3	1	2	7/2	13978.5154	0.0540
5	2	3	11/2	5	1	4	11/2	14240.6021	-0.0156
5	2	3	9/2	5	1	4	9/2	14259.7347	-0.0456
2	2	0	5/2	2	1	1	3/2	14791.5196	0.1250
2	1	1	5/2	1	1	0	3/2	14827.3960	0.0604
2	1	1	3/2	1	1	0	1/2	14827.6449	-0.0164

2	2	0	5/2	2	1	1	5/2	14831.6224	0.0483
2	2	0	3/2	2	1	1	3/2	14862.8099	-0.0714
2	1	1	3/2	1	1	0	3/2	14867.4988	0.0808
2	2	0	3/2	2	1	1	5/2	14902.9127	-0.0414
3	0	3	5/2	2	1	2	3/2	15723.6237	0.0695
3	0	3	7/2	2	1	2	5/2	15725.7672	0.0251
3	0	3	5/2	2	1	2	5/2	15743.6231	0.0827
7	2	5	15/2	7	2	6	15/2	16035.6339	0.0360
7	2	5	13/2	7	2	6	13/2	16066.0625	-0.0429
6	2	4	13/2	6	1	5	13/2	16252.2356	-0.0223
4	1	3	7/2	3	2	2	5/2	16255.7365	0.0362
4	1	3	9/2	3	2	2	7/2	16263.6950	0.0180
6	2	4	11/2	6	1	5	11/2	16276.0045	0.0647
2	1	2	5/2	1	0	1	3/2	17204.0460	0.0814
2	1	2	3/2	1	0	1	1/2	17213.9227	-0.0494
2	1	2	3/2	1	0	1	3/2	17224.0465	-0.0194

Table S2. Spectroscopic constants (A-Reduction, I^r representation) for 2-methoxy furan. The experimental constants were taken from the previous work of J.A. Beukes¹.

	Experimental	ANO0/CCSD(T)	Exp-Calc
A_0 (MHz)	7613.1668(14)	7446.93619	166.23
B_0 (MHz)	2111.50975(40)	2072.87772	38.63
C_0 (MHz)	1671.35814(32)	1639.41791	31.94
Δ_{JK} (kHz)	0.0357(59)	0.02909	0.006
Δ_J (kHz)	0.14203(89)	0.1404	0.0016
Δ_K (kHz)	2.1805(19)	2.026	0.1545
δ_j (kHz)	0.034619(24)	0.0348	-0.0002
δ_k (kHz)	0.3981(97)	0.397	0.001
Δ (uÅ ²)	-3.35	-3.25	-
σ (kHz)	67	-	-
N	532	-	-

¹J. A. Beukes, K. M. Marstokk, and H. Mollendal, J. Mol. Spec. **567-568** (2001) 19.

Figure S1 Summary of relevant reactions involved in the pyrolysis of 2-methoxy furan.

