

Table 3: Experimental frequencies (MHz) of the rotatinal spectrum of the second excited state of the ring-puckering mode of 2-azetidinone.

J	Ka	Kb	J	Ka'	Kb'	NUE(exp)	exp-calc
44	13	31	44	13	32	8404.400	0.161
19	6	13	19	6	14	8624.190	0.011
9	3	6	9	3	7	8676.530	0.234
59	17	42	59	17	43	9535.130	0.189
37	11	26	37	11	27	9600.720	0.141
30	9	21	30	9	22	10586.160	-0.016
16	5	11	16	5	12	10667.630	-0.043
23	7	16	23	7	17	11083.970	0.060
52	15	37	52	15	38	11357.520	0.090
41	12	29	41	12	30	11362.410	0.204
67	19	48	67	19	49	12271.650	0.120
13	4	9	13	4	10	12591.540	-0.040
4	1	3	4	1	4	12771.390	0.601
45	13	32	45	13	33	13256.430	0.064
27	8	19	27	8	20	13722.480	0.138
10	3	7	10	3	8	13982.240	0.105
7	2	5	7	2	6	14281.760	0.298
60	17	43	60	17	44	14761.890	0.069
38	11	27	38	11	28	15070.370	0.010
49	14	35	49	14	36	15284.730	-0.014
2	1	2	1	1	1	16225.560	0.219
17	5	12	17	5	13	16683.490	-0.049
24	7	17	24	7	18	17263.130	0.067
53	15	38	53	15	39	17449.090	-0.103
2	1	1	1	1	0	18797.130	-0.077
14	4	10	14	4	11	19132.830	0.125
35	10	25	35	10	26	19527.680	0.001
57	16	41	57	16	42	19751.630	-0.018
46	13	33	46	13	34	20178.590	0.041

11	3	8	11	3	9	20717.250	0.157
28	8	20	28	8	21	20844.230	-0.015
8	2	6	8	2	7	20867.290	0.214
21	6	15	21	6	16	20957.110	-0.111
39	11	28	39	11	29	22693.100	-0.217
50	14	36	50	14	37	22969.030	-0.025
3	1	3	2	1	2	24242.770	-0.069
18	5	13	18	5	14	24420.040	0.038
32	9	23	32	9	24	24612.620	-0.113
25	7	18	25	7	19	25415.200	-0.062
3	0	3	2	0	2	25638.190	-0.008
43	12	31	43	12	32	26034.090	-0.177
3	2	2	2	2	1	26266.920	0.128
15	4	11	15	4	12	27172.660	0.018
3	1	2	2	1	1	28087.840	-0.027
9	2	7	9	2	8	28481.240	0.088
36	10	26	36	10	27	28567.780	-0.148
12	3	9	12	3	10	28698.600	0.141
22	6	16	22	6	17	29862.410	0.162
29	8	21	29	8	22	30059.090	-0.007
4	1	4	3	1	3	32162.990	0.063
40	11	29	40	11	30	32709.250	-0.175
51	14	37	51	14	38	33242.850	-0.450
4	0	4	3	0	3	33542.820	-0.053
19	5	14	19	5	15	33711.450	-0.005
33	9	24	33	9	25	34889.400	-0.022
4	2	3	3	2	2	34896.420	-0.029
4	3	1	3	3	0	35385.430	-0.068
26	7	19	26	7	20	35469.280	0.081
4	2	2	3	2	1	36375.080	-0.105
16	4	12	16	4	13	36465.070	0.254
10	2	8	10	2	9	36830.580	0.086
4	1	3	3	1	2	37230.890	0.004

13	3	10	13	3	11	37648.090	-0.012
13	4	9	13	3	10	38022.510	-0.172
6	2	5	6	0	6	38376.280	0.108
37	10	27	37	10	28	39906.360	-0.046
5	1	5	4	1	4	39978.110	0.255
23	6	17	23	6	18	40364.790	-0.089
5	0	5	4	0	4	41113.860	-0.178
8	1	7	8	1	8	41425.570	0.193
48	13	35	48	13	36	41549.820	-0.022
15	4	11	15	3	12	41865.250	-0.190
13	3	10	13	2	11	43053.190	-0.096
5	3	3	4	3	2	44211.230	0.572
20	5	15	20	5	16	44250.820	0.019
5	3	2	4	3	1	44469.870	0.168
5	1	4	4	1	3	46148.010	-0.272
17	4	13	17	4	14	46665.090	-0.035
27	7	20	27	7	21	47149.640	-0.619
34	9	25	34	9	26	47196.630	0.002
8	2	7	8	0	8	47569.920	-0.214
6	1	6	5	1	5	47693.780	-0.292
16	5	11	16	4	12	47814.860	-0.037
15	5	10	15	4	11	50302.130	-0.153
7	3	5	7	1	6	51094.740	0.404
8	3	6	8	1	7	51125.240	-0.732
6	2	5	5	2	4	51815.670	0.015
6	3	4	5	3	3	53108.770	0.068
6	3	3	5	3	2	53770.410	-0.062
31	8	23	31	8	24	54077.630	-0.025
6	1	5	5	1	4	54747.030	-0.113
10	3	8	10	1	9	54928.590	-0.190
7	1	7	6	1	6	55328.070	0.042
21	6	15	21	5	16	55453.600	0.207
21	5	16	21	5	17	55632.990	-0.232

7	0	7	6	0	6	55840.250	0.074
49	13	36	49	13	37	56073.160	0.097
20	5	15	20	4	16	56525.390	-0.238
15	3	12	15	3	13	56967.450	-0.130
11	3	9	11	1	10	58607.110	-0.024
19	6	13	19	5	14	59290.680	0.005
42	11	31	42	11	32	59621.540	0.288
28	7	21	28	7	22	60037.590	-0.111
35	9	26	35	9	27	61153.220	0.336
7	3	5	6	3	4	61967.580	0.126
26	5	21	25	5	20	233554.330	0.270
26	7	20	25	7	19	234332.980	-0.614
30	2	29	29	2	28	233853.360	0.054
34	24	10	33	24	9	300177.910	-0.256
49	13	37	48	13	36	447367.280	0.054
56	4	52	55	4	51	447422.170	-0.557
49	11	38	48	11	37	450267.500	-0.318
49	12	38	48	12	37	443541.550	-0.177
50	26	24	49	26	23	443542.570	0.075
55	7	49	54	7	48	453208.410	0.212
51	17	34	50	17	33	461066.570	-0.029
49	12	37	48	12	36	461848.020	0.743
62	0	62	61	0	61	466021.290	-0.145