

Table 4: Experimental frequencies (MHz) of the rotatinal spectrum of the third excited state of the ring-puckering mode of 2-azetidinone.

J	KP	KO	J'	KP'	KO'	NUE(EXP)	EXP-CALC
33	10	23	33	10	24	8290.370	0.173
9	3	6	9	3	7	8735.330	-0.160
19	6	13	19	6	14	8804.050	-0.109
44	13	31	44	13	32	8858.370	0.054
55	16	39	55	16	40	8874.450	-0.068
37	11	26	37	11	27	10021.380	0.054
16	5	11	16	5	12	10831.150	-0.056
23	7	16	23	7	17	11354.640	0.477
41	12	29	41	12	30	11900.570	0.056
52	15	37	52	15	38	12053.750	0.054
13	4	9	13	4	10	12719.690	-0.058
45	13	32	45	13	33	13929.320	-0.839
10	3	7	10	3	8	14060.580	0.211
27	8	19	27	8	20	14102.870	0.029
38	11	27	38	11	28	15683.160	-0.053
2	1	2	1	1	1	16253.060	0.055
17	5	12	17	5	13	16904.850	-0.170
31	9	22	31	9	23	17048.720	0.004
24	7	17	24	7	18	17638.370	-0.167
2	1	1	1	1	0	18821.480	0.205
14	4	10	14	4	11	19295.230	-0.010
35	10	25	35	10	26	20191.560	0.042
11	3	8	11	3	9	20808.540	0.013
8	2	6	8	2	7	20889.170	-0.029
46	13	33	46	13	34	21126.440	0.179
21	6	15	21	6	16	21296.180	0.073
28	8	20	28	8	21	21359.360	0.049
39	11	28	39	11	29	23531.720	0.086
50	14	36	50	14	37	24116.470	-0.229

3	1	3	2	1	2	24284.010	0.042
18	5	13	18	5	14	24692.780	-0.086
32	9	23	32	9	24	25290.300	-0.038
3	0	3	2	0	2	25674.420	-0.029
25	7	18	25	7	19	25895.490	-0.069
3	2	2	2	2	1	26305.670	0.100
43	12	31	43	12	32	27069.860	0.066
47	13	34	47	13	35	30806.870	-0.003
36	10	26	36	10	27	29431.330	-0.065
33	9	24	33	9	25	35724.380	-0.118
3	2	1	2	2	0	26936.820	-0.028
15	4	11	15	4	12	27359.590	0.008
3	1	2	2	1	1	28123.430	-0.030
9	2	7	9	2	8	28493.640	-0.001
12	3	9	12	3	10	28793.690	0.056
22	6	16	22	6	17	30270.600	-0.071
29	8	21	29	8	22	30704.850	0.058
4	3	1	3	3	0	35438.800	-0.209
19	5	14	19	5	15	34020.320	-0.023
4	2	3	3	2	2	34947.540	-0.081
4	2	2	3	2	1	36431.470	-0.032
4	1	4	3	1	3	32217.380	0.134
4	0	4	3	0	3	33589.360	-0.171
4	1	3	3	1	2	37277.270	0.059
6	2	5	6	0	6	38171.740	-0.164
5	1	5	4	1	4	40045.320	0.101
23	6	17	23	6	18	40820.930	0.078
5	0	5	4	0	4	41172.120	0.125
17	4	13	17	4	14	46851.360	0.224
6	1	6	5	1	5	47774.780	0.239
45	12	33	45	12	34	52045.900	0.003
6	3	4	5	3	3	53187.240	-0.066
6	3	3	5	3	2	53855.470	0.185

6	1	5	5	1	4	54810.220	-0.267
31	8	23	31	8	24	54899.080	-0.210
7	1	7	6	1	6	55421.820	-0.040
7	0	7	6	0	6	55926.640	-0.001
21	5	16	21	5	17	55942.970	0.183
42	11	31	42	11	32	61068.770	0.016
49	13	36	49	13	37	57904.320	-0.587
11	3	9	11	1	10	58321.880	-0.811
5	1	4	4	1	3	46203.500	-0.519
8	2	7	8	0	8	47360.050	0.603
26	23	3	25	23	2	229387.410	0.160
36	4	32	35	4	31	298902.000	0.315
34	30	4	33	30	3	299782.470	0.035
26	12	15	25	12	14	232010.890	-1.238
30	2	29	29	2	28	234295.620	-0.029
26	8	19	25	8	18	235700.840	0.339
26	9	17	25	9	16	235408.640	-0.480
54	11	44	54	9	45	238750.770	0.059
35	28	8	34	28	7	308913.810	-0.325
35	16	20	34	16	19	312316.380	-0.071
37	5	32	36	5	31	313120.090	-0.149
37	6	32	36	6	31	313107.840	-0.771
34	30	4	33	30	3	299782.470	0.035
55	6	50	54	6	49	447416.690	0.054
51	36	16	50	36	15	450296.310	-0.032
55	6	50	54	6	49	447416.630	-0.006
50	16	34	49	16	33	454473.940	0.171
53	9	44	52	9	43	459687.430	0.002
53	31	23	52	31	22	469503.570	0.301