

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

J	KP	KO	J'	KP'	KO'	NUE(EXP)	EXP-CALC
19	6	13	19	6	14	8377.900	-0.020
59	17	42	59	17	43	8676.530	-0.115
37	11	26	37	11	27	9050.680	0.092
63	18	45	63	18	46	9834.140	0.026
30	9	21	30	9	22	10108.450	0.008
16	5	11	16	5	12	10439.740	0.018
52	15	37	52	15	38	10472.350	0.095
41	12	29	41	12	30	10662.500	0.161
23	7	16	23	7	17	10717.050	-0.021
45	13	32	45	13	33	12384.920	0.041
13	4	9	13	4	10	12408.030	0.065
27	8	19	27	8	20	13209.170	-0.095
60	17	43	60	17	44	13494.020	0.059
20	6	14	20	6	15	13513.750	0.039
75	21	54	75	21	55	13773.410	0.267
10	3	7	10	3	8	13863.970	0.157
49	14	35	49	14	36	14218.960	0.052
38	11	27	38	11	28	14263.750	0.085
31	9	22	31	9	23	15851.510	-0.044
53	15	38	53	15	39	16165.360	0.032
2	1	2	1	1	1	16190.780	-0.080
17	5	12	17	5	13	16371.580	0.051
42	12	30	42	12	31	16537.660	-0.143
24	7	17	24	7	18	16749.150	0.022
68	19	49	68	19	50	16896.980	0.134
57	16	41	57	16	42	18224.920	-0.248
35	10	25	35	10	26	18642.210	-0.059
2	1	1	1	1	0	18765.450	0.128
14	4	10	14	4	11	18896.280	0.086

46	13	33	46	13	34	18942.810	-0.143
28	8	20	28	8	21	20143.720	-0.006
61	17	44	61	17	45	20399.320	-0.207
21	6	15	21	6	16	20485.080	0.069
11	3	8	11	3	9	20574.620	0.161
8	2	6	8	2	7	20818.370	0.271
50	14	36	50	14	37	21479.430	-0.033
39	11	28	39	11	29	21580.410	-0.074
32	9	23	32	9	24	23696.150	-0.014
18	5	13	18	5	14	24030.650	0.090
3	1	3	2	1	2	24191.630	-0.100
43	12	31	43	12	32	24665.620	-0.089
25	7	18	25	7	19	24751.400	0.034
69	19	50	69	19	51	25096.180	-0.113
3	0	3	2	0	2	25592.430	-0.034
6	1	5	6	1	6	26035.670	0.176
3	2	2	2	2	1	26217.120	0.087
3	2	1	2	2	0	26841.600	-0.090
15	4	11	15	4	12	26895.110	0.091
58	16	42	58	16	43	26948.470	-0.165
36	10	26	36	10	27	27405.550	-0.020
47	13	34	47	13	35	27897.640	-0.068
3	1	2	2	1	1	28040.880	0.038
9	2	7	9	2	8	28438.230	0.157
12	3	9	12	3	10	28543.150	0.129
29	8	21	29	8	22	29172.290	0.037
22	6	16	22	6	17	29286.410	0.038
62	17	45	62	17	46	29882.440	-0.022
66	18	48	66	18	49	32949.860	-0.028
51	14	37	51	14	38	31276.320	-0.061
55	15	40	55	15	41	34801.550	-0.129
44	12	32	44	12	33	35292.830	-0.033
40	11	29	40	11	30	31271.320	0.008

33	9	24	33	9	25	33748.450	-0.118
26	7	19	26	7	20	34674.380	0.071
19	5	14	19	5	15	33263.350	-0.021
16	4	12	16	4	13	36165.060	-0.054
10	2	8	10	2	9	36806.360	0.175
13	3	10	13	3	11	37496.050	-0.080
4	2	3	3	2	2	34830.900	-0.079
4	3	1	3	3	0	35316.170	-0.204
4	2	2	3	2	1	36301.430	-0.020
4	1	4	3	1	3	32095.670	-0.019
4	0	4	3	0	3	33484.800	-0.002
4	1	3	3	1	2	37170.000	0.050
13	4	9	13	3	10	38370.230	0.337
59	16	43	59	16	44	38473.680	0.130
37	10	27	37	10	28	38480.820	0.132
6	2	5	6	0	6	38621.220	0.152
48	13	35	48	13	36	39469.740	0.027
23	6	17	23	6	18	39712.810	0.073
5	1	5	4	1	4	39894.480	-0.356
30	8	22	30	8	23	40200.640	0.019
5	0	5	4	0	4	41043.120	0.313
11	4	7	11	3	8	41361.980	-0.053
15	4	11	15	3	12	42012.660	-0.065
63	17	46	63	17	47	42292.230	0.332
7	2	6	7	0	7	42845.300	0.234
5	2	4	4	2	3	43340.000	0.432
41	11	30	41	11	31	43369.030	0.427
20	5	15	20	5	16	43771.860	-0.441
11	2	9	11	2	10	45559.840	0.139
5	1	4	4	1	3	46076.030	0.586
14	5	9	13	6	8	46248.760	1.280
27	7	20	27	7	21	46262.230	0.284
11	2	9	11	1	10	46967.150	-0.851

14	3	11	14	3	12	47079.770	-0.244
17	5	12	17	4	13	47299.930	0.302
6	1	6	5	1	5	47595.350	-0.007
56	15	41	56	15	42	48286.660	-0.405
9	1	8	9	1	9	49288.130	-0.145
15	5	10	15	4	11	50945.660	0.285
19	5	14	19	4	15	51245.870	-0.333
8	3	6	8	1	7	51566.340	-0.194
38	10	28	38	10	29	51681.520	-0.056
6	2	5	5	2	4	51720.990	0.027
16	3	13	15	5	10	52215.180	-0.227
31	8	23	31	8	24	52922.150	-0.201
6	4	3	5	4	2	52968.740	0.199
6	4	2	5	4	1	52997.190	-0.201
6	3	4	5	3	3	53007.560	0.153
9	2	8	9	0	9	53347.340	-0.052
49	13	36	49	13	37	53610.470	0.228
6	3	3	5	3	2	53660.240	-0.032
6	1	5	5	1	4	54665.230	0.058
21	5	16	21	5	17	55159.990	0.040
7	1	7	6	1	6	55213.620	0.188
10	3	8	10	1	9	55293.260	-0.074
7	0	7	6	0	6	55735.330	0.104
10	4	7	10	3	8	55953.840	-0.340
21	6	15	21	5	16	55965.100	0.096
20	5	15	20	4	16	56528.690	0.017
15	3	12	15	3	13	56887.450	-0.128
22	6	16	22	5	17	56943.520	0.195
18	4	14	18	4	15	57093.480	-0.189
20	6	14	20	5	15	57165.030	0.013
42	11	31	42	11	32	57639.540	0.228
13	5	8	13	4	9	58139.870	-0.347
11	3	9	11	1	10	58943.690	-0.153

28	7	21	28	7	22	59107.250	0.108
10	2	9	10	0	10	59281.380	0.110
35	9	26	35	9	27	59700.870	-0.080
7	2	6	6	2	5	59959.140	-0.083
19	6	13	19	5	14	60097.440	-0.139
7	6	2	6	6	1	61622.110	0.001
7	3	5	6	3	4	61850.680	-0.196
7	4	4	6	4	3	61933.520	-0.040
25	9	16	24	9	15	224839.470	-0.022
26	22	4	25	22	3	228749.380	-0.034
26	10	17	25	10	16	232816.980	0.030
26	9	18	25	9	17	233993.410	-0.038
26	8	19	25	8	18	234899.660	-0.034
27	23	4	26	23	3	237520.480	-0.053
28	4	24	27	4	23	238787.980	0.110
34	28	6	33	28	5	299083.010	-0.665
34	24	10	33	24	9	299631.560	0.038
35	14	22	34	14	21	312770.120	-0.045
35	12	23	34	12	22	315477.160	-0.065
50	25	26	49	25	25	443196.800	0.509
50	19	32	49	19	31	447609.030	0.349
50	15	36	49	15	35	454735.120	-0.945
50	14	37	49	14	36	456330.025	-0.221
51	18	34	50	18	33	458383.490	0.241
51	18	33	50	18	32	458389.060	0.294
52	10	42	51	10	41	458982.520	0.054
53	11	43	52	11	42	465868.490	-0.068
53	29	25	52	29	24	468685.320	0.797