

Rotational spectroscopy of imidazole: Accurate spectroscopic information for three vibrationally excited states and the heavy-atom isotopologues up to 295 GHz

[Supplementary Material]

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Submitted December 22, 2020. Revised March 8, 2021.

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A. Assigned Transitions for the Vibrationally Excited States and Isotopologues of Imidazole

Tables detailing the assigned transitions for each of the vibrational states and isotopologues of imidazole reported. The tables contain quantum numbers, experimental frequencies, and the observed minus calculated frequencies, and the tables are the product of the fitting procedure with the SPFIT programme [1].

Table 1: Assigned transitions of the imidazole ν_{21} state in the 75-110 and 260-295 GHz regions.

J'	K'_a	K'_c		J	K_a	K_c	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
31	23	8	←	31	23	9	77839.4322	-0.0273
31	24	8	←	31	22	9	78040.2470	-0.0133
30	22	8	←	30	22	9	78255.0156	-0.0174
30	23	8	←	30	21	9	78376.2238	0.0088
29	21	8	←	29	21	9	78614.1239	0.0084
29	22	8	←	29	20	9	78685.7024	-0.0048
28	20	8	←	28	20	9	78926.4264	0.0014
28	21	8	←	28	19	9	78967.7983	0.0145
27	19	8	←	27	19	9	79199.3172	-0.0175
27	20	8	←	27	18	9	79222.6624	-0.0066
26	18	8	←	26	18	9	79438.5171	0.0067
26	19	8	←	26	17	9	79451.3401	-0.0081
25	17	8	←	25	17	9	79648.3884	-0.0006
25	18	8	←	25	16	9	79655.2407	-0.0236
24	16	8	←	24	16	9	79832.5173	-0.0102
24	17	8	←	24	15	9	79836.1119	0.0073
23	15	8	←	23	15	9	79993.8566	0.0036
23	16	8	←	23	14	9	79995.6571	0.0006
19	12	8	←	19	10	9	80455.9727	-0.0241
18	10	8	←	18	10	9	80534.6923	0.0303
18	11	8	←	18	9	9	80534.6923	-0.0022
17	9	8	←	17	9	9	80601.7498	0.0303
17	10	8	←	17	8	9	80601.7498	0.0177
16	8	8	←	16	8	9	80658.4001	0.0190
16	9	8	←	16	7	9	80658.4001	0.0144
15	7	8	←	15	7	9	80705.8811	0.0423
15	8	8	←	15	6	9	80705.8811	0.0408
14	6	8	←	14	6	9	80745.2391	0.0451
14	7	8	←	14	5	9	80745.2391	0.0446
13	5	8	←	13	5	9	80777.4792	0.0146
13	6	8	←	13	4	9	80777.4792	0.0145
12	4	8	←	12	4	9	80803.5476	-0.0418
12	5	8	←	12	3	9	80803.5476	-0.0418

11	3	8	←	11	3	9	80824.3919	-0.0408
11	4	8	←	11	2	9	80824.3919	-0.0408
10	2	8	←	10	2	9	80840.7750	-0.0115
10	3	8	←	10	1	9	80840.7750	-0.0115
9	1	8	←	9	1	9	80853.4087	0.0358
9	2	8	←	9	0	9	80853.4087	0.0358
7	1	6	←	6	1	5	81067.1814	0.0340
7	2	6	←	6	2	5	81067.1814	0.0392
8	1	8	←	7	1	7	81095.6850	0.0396
8	0	8	←	7	0	7	81095.6850	0.0396
37	29	9	←	37	27	10	86249.8873	-0.0377
36	28	9	←	36	26	10	86667.6437	0.0099
35	27	9	←	35	25	10	87058.9204	0.0189
34	26	9	←	34	24	10	87421.6863	0.0019
33	24	9	←	33	24	10	87713.1001	-0.0005
32	23	9	←	32	23	10	88035.8820	0.0390
32	24	9	←	32	22	10	88060.4618	0.0048
31	22	9	←	31	22	10	88323.8607	-0.0055
31	23	9	←	31	21	10	88337.8897	-0.0088
30	21	9	←	30	21	10	88581.3317	0.0113
29	20	9	←	29	20	10	88811.5485	-0.0158
28	19	9	←	28	19	10	89017.3790	-0.0037
28	20	9	←	28	18	10	89019.6534	-0.0009
27	18	9	←	27	18	10	89201.1316	-0.0089
27	19	9	←	27	17	10	89202.3016	-0.0166
24	15	9	←	24	15	10	89639.4303	-0.0100
23	15	9	←	23	13	10	89753.3704	-0.0467
23	14	9	←	23	14	10	89753.3704	0.0161
22	14	9	←	22	12	10	89853.5592	-0.0162
22	13	9	←	22	13	10	89853.5592	0.0114
21	13	9	←	21	11	10	89941.2742	-0.0141
21	12	9	←	21	12	10	89941.2742	-0.0025
20	12	9	←	20	10	10	90017.7186	0.0083
20	11	9	←	20	11	10	90017.7186	0.0130
19	11	9	←	19	9	10	90083.9255	0.0055
19	10	9	←	19	10	10	90083.9255	0.0072
18	10	9	←	18	8	10	90140.9503	0.0245
18	9	9	←	18	9	10	90140.9503	0.0252
16	8	9	←	16	6	10	90231.0692	0.0390
15	7	9	←	15	5	10	90265.8533	0.0240
14	6	9	←	14	4	10	90294.8546	0.0236
13	5	9	←	13	3	10	90318.7435	-0.0028
13	4	9	←	13	4	10	90318.7435	-0.0028
12	4	9	←	12	2	10	90338.2649	0.0304
12	3	9	←	12	3	10	90338.2649	0.0304
10	2	9	←	10	0	10	90366.3317	0.0177

10	1	9	←	10	1	10	90366.3317	0.0177
7	3	5	←	6	3	4	90583.6676	0.0057
8	2	7	←	7	2	6	90609.0405	0.0315
8	1	7	←	7	1	6	90609.0405	0.0314
9	0	9	←	8	0	8	90637.7780	0.0130
9	1	9	←	8	1	8	90637.7780	0.0130
39	30	10	←	39	28	11	96081.4092	0.0109
38	29	10	←	38	27	11	96463.3243	0.0071
37	27	10	←	37	27	11	96790.8036	0.0036
36	26	10	←	36	26	11	97124.4585	-0.0083
36	27	10	←	36	25	11	97138.9102	0.0250
35	25	10	←	35	25	11	97426.8165	0.0153
35	26	10	←	35	24	11	97435.0565	-0.0311
34	24	10	←	34	24	11	97700.9639	0.0028
34	25	10	←	34	23	11	97705.6608	0.0267
33	24	10	←	33	22	11	97952.1716	0.0025
32	23	10	←	32	21	11	98176.3297	0.0015
31	22	10	←	31	20	11	98379.6688	-0.0299
27	17	10	←	27	17	11	99014.3718	0.0126
27	18	10	←	27	16	11	99014.3826	-0.0217
26	16	10	←	26	16	11	99134.9319	0.0094
26	17	10	←	26	15	11	99134.9464	0.0031
25	15	10	←	25	15	11	99242.5580	-0.0049
25	16	10	←	25	14	11	99242.5715	-0.0007
24	14	10	←	24	14	11	99338.3464	0.0131
24	15	10	←	24	13	11	99338.3595	0.0222
23	13	10	←	23	13	11	99423.2059	-0.0121
23	14	10	←	23	12	11	99423.2110	-0.0086
22	12	10	←	22	12	11	99498.1424	0.0012
22	13	10	←	22	11	11	99498.1570	0.0151
21	11	10	←	21	11	11	99563.9716	0.0017
21	12	10	←	21	10	11	99563.9856	0.0154
20	10	10	←	20	10	11	99621.5213	0.0022
20	11	10	←	20	9	11	99621.5301	0.0108
19	9	10	←	19	9	11	99671.5586	0.0033
19	10	10	←	19	8	11	99671.5684	0.0131
18	8	10	←	18	8	11	99714.8073	0.0087
18	9	10	←	18	7	11	99714.8219	0.0233
17	7	10	←	17	7	11	99751.9349	0.0090
17	8	10	←	17	6	11	99751.9480	0.0222
16	6	10	←	16	6	11	99783.5846	0.0126
16	7	10	←	16	5	11	99783.5852	0.0132
15	6	10	←	15	4	11	99810.2779	-0.0542
14	4	10	←	14	4	11	99832.7155	-0.0471
12	2	10	←	12	2	11	99866.6349	-0.0386
12	3	10	←	12	1	11	99866.6430	-0.0305

11	1	10	←	11	1	11	99879.0726	-0.0096
11	2	10	←	11	0	11	99879.0790	-0.0032
9	1	8	←	8	1	7	100150.9011	0.0038
9	2	8	←	8	2	7	100150.9011	0.0038
10	0	10	←	9	0	9	100179.8145	0.0065
10	1	10	←	9	1	9	100179.8145	0.0065
40	30	11	←	40	28	12	106202.9302	0.0242
39	28	11	←	39	28	12	106510.2889	-0.0291
38	27	11	←	38	27	12	106799.7472	-0.0311
38	28	11	←	38	26	12	106802.5407	0.0179
37	26	11	←	37	26	12	107065.0938	0.0026
37	27	11	←	37	25	12	107066.6596	0.0348
36	26	11	←	36	24	12	107308.9798	0.0025
32	22	11	←	32	20	12	108088.8674	-0.0011
31	20	11	←	31	20	12	108242.7406	0.0028
31	21	11	←	31	19	12	108242.7481	-0.0201
30	19	11	←	30	19	12	108382.4881	0.0041
30	20	11	←	30	18	12	108382.4944	-0.0042
29	18	11	←	29	18	12	108509.0371	-0.0267
29	19	11	←	29	17	12	108509.0476	-0.0230
28	17	11	←	28	17	12	108623.4300	-0.0020
28	18	11	←	28	16	12	108623.4441	0.0089
27	16	11	←	27	16	12	108726.4762	-0.0098
27	17	11	←	27	15	12	108726.4895	0.0021
26	15	11	←	26	15	12	108819.0612	-0.0096
26	16	11	←	26	14	12	108819.0695	-0.0019
25	14	11	←	25	14	12	108901.9565	-0.0268
25	15	11	←	25	13	12	108901.9671	-0.0165
24	13	11	←	24	13	12	108975.9786	0.0023
24	14	11	←	24	12	12	108975.9875	0.0111
23	12	11	←	23	12	12	109041.7470	-0.0134
23	13	11	←	23	11	12	109041.7607	0.0002
22	11	11	←	22	11	12	109100.0097	0.0015
22	12	11	←	22	10	12	109100.0162	0.0080
21	10	11	←	21	10	12	109151.3514	-0.0036
21	11	11	←	21	9	12	109151.3654	0.0104
20	9	11	←	20	9	12	109196.4040	0.0022
20	10	11	←	20	8	12	109196.4182	0.0164
19	8	11	←	19	8	12	109235.7253	0.0090
19	9	11	←	19	7	12	109235.7316	0.0153
18	7	11	←	18	7	12	109269.8289	-0.0054
18	8	11	←	18	6	12	109269.8351	0.0007
17	6	11	←	17	6	12	109299.2566	-0.0046
17	7	11	←	17	5	12	109299.2587	-0.0025
16	5	11	←	16	5	12	109324.4672	-0.0057
16	6	11	←	16	4	12	109324.4764	0.0034

15	4	11	←	15	4	12	109345.9061	-0.0100
14	4	11	←	14	2	12	109363.9781	-0.0315
13	2	11	←	13	2	12	109379.1212	-0.0233
13	3	11	←	13	1	12	109379.1227	-0.0218
12	1	11	←	12	1	12	109391.6578	-0.0274
12	2	11	←	12	0	12	109391.6898	0.0044
37	10	27	←	37	10	28	261296.7467	-0.0304
36	9	27	←	36	9	28	261333.4791	0.0103
35	8	27	←	35	8	28	261368.3192	-0.0344
33	6	27	←	33	6	28	261432.9776	0.0068
32	5	27	←	32	5	28	261462.7904	-0.0416
31	4	27	←	31	4	28	261491.1248	-0.0199
19	8	11	←	18	8	10	262158.2472	-0.0261
19	9	11	←	18	9	10	262158.2472	-0.0261
18	10	9	←	17	10	8	262166.1384	0.0117
18	9	9	←	17	9	8	262166.1384	0.0000
20	7	13	←	19	7	12	262173.5662	0.0000
20	8	13	←	19	8	12	262173.5662	0.0000
21	6	15	←	20	6	14	262197.4995	-0.0187
21	7	15	←	20	7	14	262197.4995	-0.0187
22	5	17	←	21	5	16	262225.1542	-0.0116
22	6	17	←	21	6	16	262225.1542	-0.0116
24	3	21	←	23	3	20	262284.4909	0.0125
24	4	21	←	23	4	20	262284.4909	0.0125
25	2	23	←	24	2	22	262314.6940	0.0432
25	3	23	←	24	3	22	262314.6940	0.0432
27	0	27	←	26	0	26	262374.2529	-0.0237
27	1	27	←	26	1	26	262374.2529	-0.0237
16	11	5	←	15	11	4	263305.5153	-0.0061
15	12	3	←	14	12	2	265535.5937	-0.0157
16	13	4	←	15	13	3	269833.2957	0.0019
40	12	28	←	40	12	29	270715.4815	-0.0009
39	11	28	←	39	11	29	270756.8150	-0.0021
37	9	28	←	37	9	29	270833.9187	0.0433
36	8	28	←	36	8	29	270869.7317	0.0028
34	6	28	←	34	6	29	270936.3892	-0.0064
32	4	28	←	32	4	29	270996.7487	0.0123
19	10	10	←	18	10	9	271688.9117	0.0088
19	9	10	←	18	9	9	271688.9117	0.0083
20	8	12	←	19	8	11	271691.4234	-0.0109
20	9	12	←	19	9	11	271691.4234	-0.0109
21	7	14	←	20	7	13	271710.1571	0.0104
21	8	14	←	20	8	13	271710.1571	0.0104
23	5	18	←	22	5	17	271763.7013	0.0195
23	6	18	←	22	6	17	271763.7013	0.0195
24	4	20	←	23	4	19	271793.3188	0.0257

24	5	20	←	23	5	19	271793.3188	0.0257
25	3	22	←	24	3	21	271823.4673	0.0022
25	4	22	←	24	4	21	271823.4673	0.0022
26	2	24	←	25	2	23	271853.7157	-0.0202
26	3	24	←	25	3	23	271853.7157	-0.0202
28	0	28	←	27	0	27	271913.4722	0.0304
28	1	28	←	27	1	27	271913.4722	0.0304
17	11	6	←	16	11	5	272048.1098	0.0165
38	9	29	←	38	9	30	280333.6002	0.0489
37	8	29	←	37	8	30	280370.4200	-0.0242
34	5	29	←	34	5	30	280471.3108	-0.0362
33	4	29	←	33	4	30	280501.9423	0.0384
32	3	29	←	32	3	30	280530.9890	-0.0198
31	2	29	←	31	2	30	280558.7392	0.0276
21	8	13	←	20	8	12	281225.7120	0.0144
21	9	13	←	20	9	12	281225.7120	0.0144
19	11	9	←	18	11	8	281238.0943	-0.0345
22	7	15	←	21	7	14	281246.9150	0.0040
22	8	15	←	21	8	14	281246.9150	0.0040
23	6	17	←	22	6	16	281273.2486	-0.0058
23	7	17	←	22	7	16	281273.2486	-0.0058
25	4	21	←	24	4	20	281331.8640	-0.0222
25	5	21	←	24	5	20	281331.8640	-0.0222
26	3	23	←	25	3	22	281362.2043	-0.0104
26	4	23	←	25	4	22	281362.2043	-0.0104
18	11	7	←	17	11	6	281372.9058	0.0366
27	2	25	←	26	2	24	281392.6072	0.0273
27	3	25	←	26	3	24	281392.6072	0.0273
28	1	27	←	27	1	26	281422.7040	0.0034
28	2	27	←	27	2	26	281422.7040	0.0034
29	0	29	←	28	0	28	281452.3390	-0.0233
29	1	29	←	28	1	28	281452.3390	-0.0233
17	12	5	←	16	12	4	282914.7446	-0.0239
40	10	30	←	40	10	31	289792.7940	-0.0174
39	9	30	←	39	9	31	289832.5022	0.0000
38	8	30	←	38	8	31	289870.5360	0.0338
36	6	30	←	36	6	31	289941.6595	0.0175
35	5	30	←	35	5	31	289974.8787	-0.0057
20	11	10	←	19	11	9	290753.8848	0.0047
20	10	10	←	19	10	9	290753.8848	0.0030
23	7	16	←	22	7	15	290783.7027	-0.0309
23	8	16	←	22	8	15	290783.7027	-0.0309
24	6	18	←	23	6	17	290810.9071	-0.0255
24	7	18	←	23	7	17	290810.9071	-0.0255
25	5	20	←	24	5	19	290840.1050	-0.0129
25	6	20	←	24	6	19	290840.1050	-0.0129

26	4	22	←	25	4	21	290870.2592	0.0172
26	5	22	←	25	5	21	290870.2592	0.0172
28	2	26	←	27	2	25	290931.1767	0.0040
28	3	26	←	27	3	25	290931.1767	0.0040
29	1	28	←	28	1	27	290961.3575	0.0120
29	2	28	←	28	2	27	290961.3575	0.0120
18	13	6	←	17	13	5	291034.1370	-0.0159
18	12	6	←	17	12	5	291290.2579	-0.0338

Table 2: Assigned transitions of the imidazole ν_{20} state in the 75-110 and 260-295 GHz regions.

J'	K'_a	K'_c		J	K_a	K_c	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
23	15	8	←	23	15	9	79870.5726	-0.0296
23	16	8	←	23	14	9	79872.1524	-0.0269
20	13	8	←	20	11	9	80228.0585	-0.0249
19	12	8	←	19	10	9	80316.6657	-0.0113
18	11	8	←	18	9	9	80392.6872	-0.0067
18	10	8	←	18	10	9	80392.6872	0.0217
17	10	8	←	17	8	9	80457.4527	-0.0038
17	9	8	←	17	9	9	80457.4527	0.0071
16	9	8	←	16	7	9	80512.2082	0.0135
16	8	8	←	16	8	9	80512.2082	0.0175
15	8	8	←	15	6	9	80558.0815	0.0308
15	7	8	←	15	7	9	80558.0815	0.0321
13	6	8	←	13	4	9	80627.2591	-0.0157
13	5	8	←	13	5	9	80627.2591	-0.0156
6	3	4	←	5	3	3	81019.2827	-0.0214
6	2	4	←	5	2	3	81036.0256	-0.0262
30	21	9	←	30	21	10	88472.9542	-0.0052
29	20	9	←	29	20	10	88694.7421	0.0091
28	19	9	←	28	19	10	88893.1330	0.0200
27	19	9	←	27	17	10	89071.3161	-0.0187
25	17	9	←	25	15	10	89369.0056	-0.0194
23	15	9	←	23	13	10	89603.3202	-0.0239
23	14	9	←	23	14	10	89603.3202	0.0299
21	13	9	←	21	11	10	89784.7901	-0.0109
21	12	9	←	21	12	10	89784.7901	-0.0009
20	12	9	←	20	10	10	89858.6457	0.0155
20	11	9	←	20	11	10	89858.6457	0.0195
19	11	9	←	19	9	10	89922.6004	-0.0018
19	10	9	←	19	10	10	89922.6004	-0.0002
18	10	9	←	18	8	10	89977.6867	-0.0015
18	9	9	←	18	9	10	89977.6867	-0.0010
17	9	9	←	17	7	10	90024.8087	0.0124
17	8	9	←	17	8	10	90024.8087	0.0125
16	8	9	←	16	6	10	90064.7989	0.0244
16	7	9	←	16	7	10	90064.7989	0.0245
14	6	9	←	14	4	10	90126.4384	-0.0154
14	5	9	←	14	5	10	90126.4384	-0.0154
11	3	9	←	11	1	10	90183.5544	-0.0295
11	2	9	←	11	2	10	90183.5544	-0.0295
10	2	9	←	10	0	10	90195.5872	-0.0042
10	1	9	←	10	1	10	90195.5872	-0.0042
36	27	10	←	36	25	11	97045.5643	-0.0153

35	26	10	←	35	24	11	97331.1868	0.0085
34	24	10	←	34	24	11	97588.0967	0.0032
34	25	10	←	34	23	11	97592.0642	0.0162
33	23	10	←	33	23	11	97827.6329	0.0241
32	22	10	←	32	22	11	98044.8369	0.0207
32	23	10	←	32	21	11	98046.0224	0.0241
27	18	10	←	27	16	11	98854.7821	-0.0105
27	17	10	←	27	17	11	98854.7821	0.0275
26	17	10	←	26	15	11	98971.1956	0.0039
26	16	10	←	26	16	11	98971.1956	0.0215
25	16	10	←	25	14	11	99075.1371	-0.0041
25	15	10	←	25	15	11	99075.1371	0.0036
24	15	10	←	24	13	11	99167.6499	0.0034
24	14	10	←	24	14	11	99167.6499	0.0068
23	14	10	←	23	12	11	99249.6485	-0.0029
23	13	10	←	23	13	11	99249.6485	-0.0015
22	13	10	←	22	11	11	99322.0322	-0.0111
22	12	10	←	22	12	11	99322.0322	-0.0106
21	12	10	←	21	10	11	99385.6461	-0.0106
21	11	10	←	21	11	11	99385.6461	-0.0104
20	11	10	←	20	9	11	99441.2872	0.0109
20	10	10	←	20	10	11	99441.2872	0.0110
19	10	10	←	19	8	11	99489.6393	-0.0013
19	9	10	←	19	9	11	99489.6393	-0.0013
18	9	10	←	18	7	11	99531.4567	0.0122
18	8	10	←	18	8	11	99531.4567	0.0122
17	8	10	←	17	6	11	99567.3360	-0.0043
17	7	10	←	17	7	11	99567.3360	-0.0043
16	7	10	←	16	5	11	99597.9615	0.0205
16	6	10	←	16	6	11	99597.9615	0.0205
15	6	10	←	15	4	11	99623.8585	0.0376
15	5	10	←	15	5	11	99623.8585	0.0376
11	2	10	←	11	0	11	99690.3282	-0.0089
11	1	10	←	11	1	11	99690.3282	-0.0089
37	26	11	←	37	26	12	106938.7060	-0.0160
37	27	11	←	37	25	12	106939.9851	-0.0116
36	26	11	←	36	24	12	107173.6714	-0.0149
33	23	11	←	33	21	12	107762.8667	-0.0098
32	22	11	←	32	20	12	107926.1156	-0.0119
31	21	11	←	31	19	12	108074.7330	0.0384
30	20	11	←	30	18	12	108209.5931	-0.0157
30	19	11	←	30	19	12	108209.5987	0.0019
29	19	11	←	29	17	12	108331.8418	0.0023
29	18	11	←	29	18	12	108331.8418	0.0079
28	18	11	←	28	16	12	108442.3037	0.0043
28	17	11	←	28	17	12	108442.3037	0.0068

27	17	11	←	27	15	12	108541.8473	-0.0008
27	16	11	←	27	16	12	108541.8473	0.0002
26	16	11	←	26	14	12	108631.2770	-0.0203
26	15	11	←	26	15	12	108631.2770	-0.0198
25	15	11	←	25	13	12	108711.4151	0.0022
25	14	11	←	25	14	12	108711.4151	0.0024
24	14	11	←	24	12	12	108782.9032	-0.0156
24	13	11	←	24	13	12	108782.9032	-0.0155
23	13	11	←	23	11	12	108846.4826	-0.0172
23	12	11	←	23	12	12	108846.4826	-0.0172
21	11	11	←	21	9	12	108952.4118	-0.0311
21	10	11	←	21	10	12	108952.4118	-0.0311
20	10	11	←	20	8	12	108995.9878	-0.0091
20	9	11	←	20	9	12	108995.9878	-0.0091
19	9	11	←	19	7	12	109034.0024	-0.0110
19	8	11	←	19	8	12	109034.0024	-0.0110
17	10	7	←	16	10	6	262134.5112	0.0355
36	8	28	←	36	8	29	270360.8945	0.0349
38	9	29	←	38	9	30	279807.6865	0.0079
37	8	29	←	37	8	30	279843.5293	-0.0029
20	9	11	←	19	9	10	281131.2864	0.0388
20	10	11	←	19	10	10	281131.2864	0.0388
21	8	13	←	20	8	12	281163.5916	-0.0287
21	9	13	←	20	9	12	281163.5916	-0.0287
22	7	15	←	21	7	14	281207.3953	-0.0157
22	8	15	←	21	8	14	281207.3953	-0.0157
23	6	17	←	22	6	16	281256.1850	-0.0027
23	7	17	←	22	7	16	281256.1850	-0.0027
24	5	19	←	23	5	18	281307.3629	0.0369
24	6	19	←	23	6	18	281307.3629	0.0369
25	4	21	←	24	4	20	281359.5807	-0.0149
25	5	21	←	24	5	20	281359.5807	-0.0149
39	9	30	←	39	9	31	289288.5855	-0.0181
36	6	30	←	36	6	31	289394.6870	-0.0125
21	9	12	←	20	9	11	290665.9842	0.0072
21	10	12	←	20	10	11	290665.9842	0.0072
22	8	14	←	21	8	13	290702.9478	-0.0333
22	9	14	←	21	9	13	290702.9478	-0.0333
23	7	16	←	22	7	15	290748.5972	-0.0095
23	8	16	←	22	8	15	290748.5972	-0.0095
24	6	18	←	23	6	17	290798.2263	0.0086
24	7	18	←	23	7	17	290798.2263	0.0086

Table 3: Assigned transitions of the imidazole ν_{19} state in the 75-110 and 260-295 GHz regions.

J'	K'_a	K'_c		J	K_a	K_c	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
20	12	8	←	20	12	9	80176.1392	-0.0342
19	12	8	←	19	10	9	80272.9887	0.0024
18	11	8	←	18	9	9	80355.8415	0.0359
17	10	8	←	17	8	9	80426.3544	0.0371
16	9	8	←	16	7	9	80485.9052	0.0318
9	2	8	←	9	0	9	80690.3406	0.0262
6	3	4	←	5	3	3	81017.0844	-0.0331
8	0	8	←	7	0	7	81122.1879	0.0412
8	1	8	←	7	1	7	81122.1879	0.0412
33	24	9	←	33	24	10	87380.7021	-0.0048
32	23	9	←	32	23	10	87724.5069	0.0085
24	16	9	←	24	14	10	89420.9309	-0.0035
23	15	9	←	23	13	10	89540.8076	0.0217
22	14	9	←	22	12	10	89646.2153	0.0319
20	12	9	←	20	10	10	89818.8073	0.0312
19	11	9	←	19	9	10	89888.3634	0.0235
19	10	9	←	19	10	10	89888.37	0.0324
18	10	9	←	18	8	10	89948.2285	0.031
18	9	9	←	18	9	10	89948.2336	0.0369
16	8	9	←	16	6	10	90042.7542	0.0386
16	7	9	←	16	7	10	90042.7577	0.0422
14	5	9	←	14	5	10	90109.5332	0.0035
14	6	9	←	14	4	10	90109.5362	0.0066
32	22	10	←	32	22	11	97885.7325	-0.0144
32	23	10	←	32	21	11	97887.551	-0.0292
29	19	10	←	29	19	11	98470.997	-0.0448
29	20	10	←	29	18	11	98471.3388	0.0433
28	19	10	←	28	17	11	98629.0051	-0.0288
27	18	10	←	27	16	11	98770.6819	0.0004
26	17	10	←	26	15	11	98897.5362	0.0319
25	16	10	←	25	14	11	99010.7093	0.0204
24	15	10	←	24	13	11	99111.3791	0.0322
23	14	10	←	23	12	11	99200.5549	0.0345
21	12	10	←	21	10	11	99348.2985	0.0324
21	11	10	←	21	11	11	99348.3072	0.0415
20	11	10	←	20	9	11	99408.6063	-0.0128
20	10	10	←	20	10	11	99408.6117	-0.0073
19	10	10	←	19	8	11	99461.0487	-0.0086
19	9	10	←	19	9	11	99461.0568	-0.0005
18	9	10	←	18	7	11	99506.3453	0.0029
18	8	10	←	18	8	11	99506.3518	0.0094
17	8	10	←	17	6	11	99545.1976	0.0081

17	7	10	←	17	7	11	99545.2021	0.0127
16	7	10	←	16	5	11	99578.2878	0.0183
16	6	10	←	16	6	11	99578.2965	0.027
15	6	10	←	15	4	11	99606.1664	-0.0446
15	5	10	←	15	5	11	99606.1726	-0.0384
14	4	10	←	14	4	11	99629.5651	-0.0364
14	5	10	←	14	3	11	99629.5717	-0.0298
8	3	6	←	7	3	5	100112.503	-0.0033
8	2	6	←	7	2	5	100112.503	-0.039
6	5	1	←	5	5	0	105415.3	-0.0218
34	23	11	←	34	23	12	107431.051	0.0609
32	21	11	←	32	21	12	107804.743	-0.0134
31	21	11	←	31	19	12	107966.762	-0.0361
31	20	11	←	31	20	12	107966.766	0.0094
30	20	11	←	30	18	12	108113.76	-0.0138
30	19	11	←	30	19	12	108113.771	0.0169
29	19	11	←	29	17	12	108246.809	-0.0358
29	18	11	←	29	18	12	108246.816	-0.0204
28	18	11	←	28	16	12	108367.033	0.009
28	17	11	←	28	17	12	108367.041	0.0218
26	16	11	←	26	14	12	108572.442	-0.0129
26	15	11	←	26	15	12	108572.45	-0.0043
25	15	11	←	25	13	12	108659.429	-0.0197
25	14	11	←	25	14	12	108659.435	-0.0138
24	14	11	←	24	12	12	108737.025	-0.0153
24	13	11	←	24	13	12	108737.029	-0.0114
23	13	11	←	23	11	12	108805.965	-0.0183
23	12	11	←	23	12	12	108805.971	-0.0123
22	12	11	←	22	10	12	108866.978	-0.0104
22	11	11	←	22	11	12	108866.981	-0.007
21	11	11	←	21	9	12	108920.714	-0.0139
21	10	11	←	21	10	12	108920.72	-0.0079
20	10	11	←	20	8	12	108967.834	-0.0029
20	9	11	←	20	9	12	108967.839	0.002
17	7	11	←	17	5	12	109075.17	-0.0452
17	6	11	←	17	6	12	109075.173	-0.0415
16	5	11	←	16	5	12	109101.425	-0.0456
42	15	27	←	42	15	28	260553.363	0.0065
34	7	27	←	34	7	28	260873.203	-0.0453
30	3	27	←	30	3	28	260989.661	-0.0104
29	2	27	←	29	2	28	261014.977	0.0033
18	9	9	←	17	9	8	262069.445	0.0019
19	8	11	←	18	8	10	262082.937	-0.0315
19	9	11	←	18	9	10	262082.937	-0.0315
20	7	13	←	19	7	12	262120.969	0.0268
20	8	13	←	19	8	12	262120.969	0.0268

17	10	7	←	16	10	6	262142.721	-0.0233
21	6	15	←	20	6	14	262168.109	0.0503
21	7	15	←	20	7	14	262168.109	0.0503
22	5	17	←	21	5	16	262219.066	-0.0288
22	6	17	←	21	6	16	262219.066	-0.0288
23	4	19	←	22	4	18	262271.903	-0.0188
23	5	19	←	22	5	18	262271.903	-0.0188
43	15	28	←	43	15	29	270030.566	-0.0187
39	11	28	←	39	11	29	270209.148	0.0312
38	10	28	←	38	10	29	270248.722	0.0086
36	8	28	←	36	8	29	270322.346	-0.0076
33	5	28	←	33	5	29	270419.937	0.023
32	4	28	←	32	4	29	270449.2	-0.0422
19	10	10	←	18	10	9	271595.863	0.0353
19	9	10	←	18	9	9	271595.863	0.0345
21	7	14	←	20	7	13	271661.907	0.0176
21	8	14	←	20	8	13	271661.907	0.0176
28	0	28	←	27	0	27	272030.363	-0.0332
28	1	28	←	27	1	27	272030.363	-0.0332
40	11	29	←	40	11	30	279687.966	-0.0117
38	9	29	←	38	9	30	279767.153	0.035
33	4	29	←	33	4	30	279935.105	-0.0287
32	3	29	←	32	3	30	279964.07	-0.0135
21	8	13	←	20	8	12	281158.866	0.0206
21	9	13	←	20	9	12	281158.866	0.0206
22	7	15	←	21	7	14	281203.084	0.0422
22	8	15	←	21	8	14	281203.084	0.0422
24	5	19	←	23	5	18	281304.87	0.0158
24	6	19	←	23	6	18	281304.87	0.0158
25	4	21	←	24	4	20	281358.31	0.0253
25	5	21	←	24	5	20	281358.31	0.0253
26	3	23	←	25	3	22	281412.274	0.0201
26	4	23	←	25	4	22	281412.274	0.0201
39	9	30	←	39	9	31	289247.015	-0.0422
36	6	30	←	36	6	31	289355.933	0.021
35	5	30	←	35	5	31	289389.064	0.0634
33	3	30	←	33	3	31	289450.701	0.0094
20	11	10	←	19	11	9	290647.354	-0.0252
20	10	10	←	19	10	9	290647.354	-0.0274
21	9	12	←	20	9	11	290661.253	-0.0413
21	10	12	←	20	10	11	290661.253	-0.0413
23	8	16	←	22	8	15	290744.22	-0.0458
24	6	18	←	23	6	17	290794.769	-0.0121
24	7	18	←	23	7	17	290794.769	-0.0121
25	5	20	←	24	5	19	290847.441	0.0136

25 6 20 ← 24 6 19 290847.441 0.0136

Table 4: Assigned transitions of the imidazole $^{15}\text{N}(1)$ isotopologue in the 12-15.5, 18-26, 75-110 and 260-295 GHz regions. For transitions in the 75-110 and 260-295 GHz regions, the F quantum number becomes redundant due to the absence of hyperfine structure, and the F value is set to the value of the J quantum number.

J'	K'_a	K'_c	F'		J	K_a	K_c	F	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
1	0	1	1	←	0	0	0	1	13903.4469	0.0074
1	0	1	2	←	0	0	0	1	13904.5078	0.0071
1	0	1	0	←	0	0	0	1	13906.0996	0.007
2	2	1	3	←	2	0	2	3	14977.5079	-0.0267
2	1	2	2	←	1	1	1	1	23335.7907	0.0256
2	1	2	2	←	1	1	1	2	23336.1553	0.0085
2	1	2	3	←	1	1	1	2	23336.8957	0.0209
2	1	2	1	←	1	1	1	1	23336.8957	-0.0018
2	1	2	1	←	1	1	1	0	23337.8723	0.0203
3	1	2	3	←	3	1	3	4	23449.6798	-0.0615
3	1	2	2	←	3	1	3	2	23449.6798	0.0036
3	1	2	4	←	3	1	3	4	23449.9774	0.0333
3	1	2	3	←	3	1	3	3	23450.7201	0.0107
2	0	2	1	←	1	0	1	0	23801.9155	0.017
2	0	2	2	←	1	0	1	2	23802.2368	0.0026
30	23	8	30	←	30	21	9	30	75454.9458	-0.035
28	20	8	28	←	28	20	9	28	75625.2086	0.0165
29	22	8	29	←	29	20	9	29	75892.3096	0.0137
28	21	8	28	←	28	19	9	28	76360.2905	0.0058
27	19	8	27	←	27	19	9	27	76402.6811	0.0246
27	20	8	27	←	27	18	9	27	76827.771	0.0259
26	18	8	26	←	26	18	9	26	77035.8467	0.0261
26	19	8	26	←	26	17	9	26	77274.6718	0.0027
25	17	8	25	←	25	17	9	25	77559.1109	0.014
25	18	8	25	←	25	16	9	25	77689.3622	0.0217
18	17	2	18	←	18	15	3	18	77907.9757	0.0362
24	16	8	24	←	24	16	9	24	77997.114	0.0213
24	17	8	24	←	24	15	9	24	78065.9341	0.0257
23	15	8	23	←	23	15	9	23	78367.3245	0.0198
23	16	8	23	←	23	14	9	23	78402.4713	0.0077
22	15	8	22	←	22	13	9	22	78699.5562	-0.0354
21	13	8	21	←	21	13	9	21	78951.1485	0.0209
21	14	8	21	←	21	12	9	21	78959.3074	-0.0316
20	12	8	20	←	20	12	9	20	79180.8549	0.0707
20	13	8	20	←	20	11	9	20	79184.5372	0.0243
19	11	8	19	←	19	11	9	19	79376.6608	0.0442
19	12	8	19	←	19	10	9	19	79378.2306	-0.0009
18	10	8	18	←	18	10	9	18	79542.9379	-0.0547
18	11	8	18	←	18	9	9	18	79543.6476	-0.0086

37	30	8	37	←	37	28	9	37	79665.046	0.0857
16	8	8	16	←	16	8	9	16	79801.6167	0.049
16	9	8	16	←	16	7	9	16	79801.6167	-0.0439
11	3	8	11	←	11	3	9	11	80141.2671	-0.0666
11	4	8	11	←	11	2	9	11	80141.2671	-0.0667
10	2	8	10	←	10	2	9	10	80173.7419	-0.1064
10	3	8	10	←	10	1	9	10	80173.7419	-0.1065
6	2	4	6	←	5	2	3	5	80233.8761	0.0559
5	3	2	5	←	4	3	1	4	81443.4542	-0.0348
34	25	9	34	←	34	25	10	34	82045.5377	0.0344
37	29	9	37	←	37	27	10	37	82631.8262	-0.0755
38	30	9	38	←	38	28	10	38	82682.4194	-0.0452
36	28	9	36	←	36	26	10	36	82850.4009	0.0078
39	31	9	39	←	39	29	10	39	83121.511	-0.0219
33	24	9	33	←	33	24	10	33	83242.5813	0.0763
35	27	9	35	←	35	25	10	35	83243.1653	0.0049
34	26	9	34	←	34	24	10	34	83737.891	0.0185
32	23	9	32	←	32	23	10	32	84214.032	0.0306
33	25	9	33	←	33	23	10	33	84281.456	0.0102
32	24	9	32	←	32	22	10	32	84836.6135	0.0421
31	22	9	31	←	31	22	10	31	85014.2672	-0.0055
31	23	9	31	←	31	21	10	31	85378.3753	0.0198
30	21	9	30	←	30	21	10	30	85683.6216	0.0092
30	22	9	30	←	30	20	10	30	85891.3467	0.0515
29	20	9	29	←	29	20	10	29	86251.1723	-0.0681
29	21	9	29	←	29	19	10	29	86366.7043	0.0026
28	19	9	28	←	28	19	10	28	86738.1593	0.0353
28	20	9	28	←	28	18	10	28	86800.6185	0.0013
27	18	9	27	←	27	18	10	27	87159.3541	0.0315
27	19	9	27	←	27	17	10	27	87192.2428	0.0354
26	17	9	26	←	26	17	10	26	87525.7806	-0.0035
26	18	9	26	←	26	16	10	26	87542.5557	-0.0241
25	16	9	25	←	25	16	10	25	87845.6502	0.0041
25	17	9	25	←	25	15	10	25	87853.9231	-0.0325
24	16	9	24	←	24	14	10	24	88129.1198	0.005
23	15	9	23	←	23	13	10	23	88371.052	0.0054
22	14	9	22	←	22	12	10	22	88582.7783	0.0381
21	12	9	21	←	21	12	10	21	88766.7243	-0.0033
20	12	9	20	←	20	10	10	20	88926.6885	-0.0549
20	12	9	20	←	20	10	10	20	88926.6885	-0.0549
19	11	9	19	←	19	9	10	19	89064.2593	-0.016
19	10	9	19	←	19	10	10	19	89064.2593	0.0368
18	9	9	18	←	18	9	10	18	89181.984	0.0096
18	9	9	18	←	18	9	10	18	89181.984	0.0096
18	10	9	18	←	18	8	10	18	89181.984	-0.0092
39	29	10	39	←	39	29	11	39	89187.9968	0.0178

17	9	9	17	←	17	7	10	17	89282.021	-0.023
17	8	9	17	←	17	8	10	17	89282.021	-0.0167
16	8	9	16	←	16	6	10	16	89366.3936	-0.0126
16	7	9	16	←	16	7	10	16	89366.3936	-0.0106
9	0	9	9	←	8	0	8	8	89608.72	0.0006
9	1	9	9	←	8	1	8	8	89608.72	0.0006
8	1	7	8	←	7	1	6	7	89614.6387	-0.0091
8	2	7	8	←	7	2	6	7	89614.6387	-0.0077
7	3	5	7	←	6	3	4	6	89627.0034	0.0484
19	17	2	19	←	19	15	5	19	90075.639	-0.0639
41	32	10	41	←	41	30	11	41	90456.4054	-0.0102
38	28	10	38	←	38	28	11	38	90621.0175	0.0196
40	31	10	40	←	40	29	11	40	90867.5732	0.0326
39	30	10	39	←	39	28	11	39	91408.367	-0.0312
37	27	10	37	←	37	27	11	37	91793.1766	-0.0562
38	29	10	38	←	38	27	11	38	92018.3779	0.0199
37	28	10	37	←	37	26	11	37	92653.8635	0.0169
36	26	10	36	←	36	26	11	36	92766.174	0.0464
35	25	10	35	←	35	25	11	35	93586.1098	0.0393
35	26	10	35	←	35	24	11	35	93892.1281	-0.0068
45	34	11	45	←	45	34	12	45	94040.6889	0.0231
34	24	10	34	←	34	24	11	34	94287.2301	0.0692
34	25	10	34	←	34	23	11	34	94463.7983	-0.0064
33	23	10	33	←	33	23	11	33	94894.1223	0.0157
33	24	10	33	←	33	22	11	33	94993.778	-0.0063
32	22	10	32	←	32	22	11	32	95424.7303	-0.0142
32	23	10	32	←	32	21	11	32	95479.6752	-0.0199
31	21	10	31	←	31	21	11	31	95892.0526	0.018
31	22	10	31	←	31	20	11	31	95921.6103	0.0094
30	20	10	30	←	30	20	11	30	96305.5505	0.0073
30	21	10	30	←	30	19	11	30	96321.0867	0.0355
29	19	10	29	←	29	19	11	29	96672.5058	0.0018
29	20	10	29	←	29	18	11	29	96680.3916	-0.0311
28	19	10	28	←	28	17	11	28	97002.4922	0.0083
27	17	10	27	←	27	17	11	27	97288.2356	0.0037
21	19	2	21	←	21	17	5	21	97425.187	0.0275
26	17	10	26	←	26	15	11	26	97546.1892	-0.003
24	14	10	24	←	24	14	11	24	97974.2606	0.0861
24	15	10	24	←	24	13	11	24	97974.2606	-0.0857
23	14	10	23	←	23	12	11	23	98151.3397	-0.0331
23	13	10	23	←	23	13	11	23	98151.3397	0.0382
21	12	10	21	←	21	10	11	21	98442.3675	-0.0006
21	11	10	21	←	21	11	11	21	98442.3675	0.01
20	11	10	20	←	20	9	11	20	98560.2601	-0.0076
20	10	10	20	←	20	10	11	20	98560.2601	-0.0038
19	10	10	19	←	19	8	11	19	98662.1616	0.0132

19	9	10	19	←	19	9	11	19	98662.1616	0.0144
18	8	10	18	←	18	8	11	18	98749.6307	-0.0021
18	9	10	18	←	18	7	11	18	98749.6307	-0.0025
17	8	10	17	←	17	6	11	17	98824.1455	-0.0831
17	7	10	17	←	17	7	11	17	98824.1455	-0.083
16	6	10	16	←	16	6	11	16	98887.3638	0.0295
16	7	10	16	←	16	5	11	16	98887.3638	0.0294
13	3	10	13	←	13	3	11	13	99020.1435	-0.1089
13	4	10	13	←	13	2	11	13	99020.1435	-0.1089
7	4	4	7	←	6	4	3	6	99035.2479	0.0194
10	0	10	10	←	9	0	9	9	99040.6147	-0.0267
10	1	10	10	←	9	1	9	9	99040.6147	-0.0267
9	1	8	9	←	8	1	7	8	99046.2697	0.0047
9	2	8	9	←	8	2	7	8	99046.2697	0.0048
42	31	11	42	←	42	31	12	42	99158.002	-0.0174
41	30	11	41	←	41	30	12	41	100308.993	-0.0052
6	4	2	6	←	5	4	1	5	100374.1844	-0.0009
41	31	11	41	←	41	29	12	41	101013.6536	-0.0414
40	29	11	40	←	40	29	12	40	101283.857	0.0158
40	30	11	40	←	40	28	12	40	101710.6576	-0.0363
39	28	11	39	←	39	28	12	39	102121.7516	-0.0291
38	27	11	38	←	38	27	12	38	102851.5228	-0.002
38	28	11	38	←	38	26	12	38	102999.2288	-0.0347
37	26	11	37	←	37	26	12	37	103493.918	-0.0106
37	27	11	37	←	37	25	12	37	103578.2829	-0.0034
36	25	11	36	←	36	25	12	36	104064.1735	0
36	26	11	36	←	36	24	12	36	104111.3615	0.0048
34	24	11	34	←	34	22	12	34	105043.9304	0.0184
33	22	11	33	←	33	22	12	33	105440.5283	-0.0349
33	23	11	33	←	33	21	12	33	105447.7798	-0.0196
32	22	11	32	←	32	20	12	32	105813.7263	0.0454
31	20	11	31	←	31	20	12	31	106142.4967	-0.0241
30	19	11	30	←	30	19	12	30	106441.6456	-0.0275
30	20	11	30	←	30	18	12	30	106442.5478	-0.0152
28	18	11	28	←	28	16	12	28	106951.7746	0.0112
27	17	11	27	←	27	15	12	27	107167.3956	-0.0559
27	16	11	27	←	27	16	12	27	107167.3956	0.0281
26	15	11	26	←	26	15	12	26	107360.0473	0.034
26	16	11	26	←	26	14	12	26	107360.0473	-0.0017
23	13	11	23	←	23	11	12	23	107818.0412	0.0056
23	12	11	23	←	23	12	12	23	107818.0412	0.0077
22	11	11	22	←	22	11	12	22	107936.3812	0.0295
22	12	11	22	←	22	10	12	22	107936.3812	0.0288
21	11	11	21	←	21	9	12	21	108040.0042	-0.0005
21	10	11	21	←	21	10	12	21	108040.0042	-0.0002
20	9	11	20	←	20	9	12	20	108130.3103	-0.0363

20	10	11	20	←	20	8	12	20	108130.3103	-0.0364
18	8	11	18	←	18	6	12	18	108276.0577	-0.0208
18	7	11	18	←	18	7	12	18	108276.0577	-0.0208
17	6	11	17	←	17	6	12	17	108333.7309	-0.0267
17	7	11	17	←	17	5	12	17	108333.7309	-0.0267
11	0	11	11	←	10	0	10	10	108472.4683	-0.0139
11	1	11	11	←	10	1	10	10	108472.4683	-0.0139
10	1	9	10	←	9	1	8	9	108477.9242	0.0171
10	2	9	10	←	9	2	8	9	108477.9242	0.0171
9	2	7	9	←	8	2	6	8	108486.2243	-0.0196
9	3	7	9	←	8	3	6	8	108486.2243	-0.0097
28	0	28	28	←	27	0	27	27	268792.6901	-0.0636
28	0	28	28	←	27	1	27	27	268792.6901	-0.0636
28	1	28	28	←	27	1	27	27	268792.6901	-0.0636
28	1	28	28	←	27	0	27	27	268792.6901	-0.0636
27	2	26	27	←	26	1	25	26	268797.2453	-0.0589
27	1	26	27	←	26	1	25	26	268797.2453	-0.0589
27	2	26	27	←	26	2	25	26	268797.2453	-0.0589
27	1	26	27	←	26	2	25	26	268797.2453	-0.0589
26	3	24	26	←	25	2	23	25	268801.4814	-0.0228
26	2	24	26	←	25	3	23	25	268801.4814	-0.0228
26	2	24	26	←	25	2	23	25	268801.4814	-0.0228
26	3	24	26	←	25	3	23	25	268801.4814	-0.0228
22	6	16	22	←	21	7	15	21	268824.987	-0.0522
22	6	16	22	←	21	6	15	21	268824.987	-0.0522
22	7	16	22	←	21	6	15	21	268824.987	-0.0522
22	7	16	22	←	21	7	15	21	268824.987	-0.0522
21	8	14	21	←	20	7	13	20	268839.9051	-0.0244
21	8	14	21	←	20	8	13	20	268839.9051	-0.0244
21	7	14	21	←	20	7	13	20	268839.9051	-0.0244
21	7	14	21	←	20	8	13	20	268839.9051	-0.0244
52	24	29	52	←	52	22	30	52	276893.4895	-0.0221
52	23	29	52	←	52	23	30	52	276893.4895	-0.0221
49	20	29	49	←	49	20	30	49	277198.1771	-0.0184
49	21	29	49	←	49	19	30	49	277198.1771	-0.0184
27	3	25	27	←	26	3	24	26	278230.323	0.0332
27	2	25	27	←	26	2	24	26	278230.323	0.0332
27	3	25	27	←	26	2	24	26	278230.323	0.0332
27	2	25	27	←	26	3	24	26	278230.323	0.0332
25	5	21	25	←	24	4	20	24	278238.7878	0.027
25	4	21	25	←	24	5	20	24	278238.7878	0.027
25	5	21	25	←	24	5	20	24	278238.7878	0.027
25	4	21	25	←	24	4	20	24	278238.7878	0.027
24	5	19	24	←	23	5	18	23	278244.2679	0.0091
24	6	19	24	←	23	5	18	23	278244.2679	0.0091
24	6	19	24	←	23	6	18	23	278244.2679	0.0091

24	5	19	24	←	23	6	18	23	278244.2679	0.0091
32	3	29	32	←	32	3	30	32	278266.637	0.0436
32	3	29	32	←	32	2	30	32	278266.637	0.0436
32	4	29	32	←	32	3	30	32	278266.637	0.0436
32	4	29	32	←	32	2	30	32	278266.637	0.0436
30	0	30	30	←	29	1	29	29	287650.2242	-0.0061
30	1	30	30	←	29	0	29	29	287650.2242	-0.0061
30	1	30	30	←	29	1	29	29	287650.2242	-0.0061
30	0	30	30	←	29	0	29	29	287650.2242	-0.0061
29	2	28	29	←	28	1	27	28	287654.8371	0.0941
29	1	28	29	←	28	1	27	28	287654.8371	0.0941
29	1	28	29	←	28	2	27	28	287654.8371	0.0941
29	2	28	29	←	28	2	27	28	287654.8371	0.0941
27	4	24	27	←	26	3	23	26	287662.7985	0.0239
27	4	24	27	←	26	4	23	26	287662.7985	0.0239
27	3	24	27	←	26	4	23	26	287662.7985	0.0239
27	3	24	27	←	26	3	23	26	287662.7985	0.0239
25	6	20	25	←	24	6	19	24	287672.0866	-0.0177
25	6	20	25	←	24	5	19	24	287672.0866	-0.0177
25	5	20	25	←	24	5	19	24	287672.0866	-0.0177
25	5	20	25	←	24	6	19	24	287672.0866	-0.0177
22	9	14	22	←	21	9	13	21	287710.072	0.0206
22	9	14	22	←	21	8	13	21	287710.072	0.0206
22	8	14	22	←	21	8	13	21	287710.072	0.0206
22	8	14	22	←	21	9	13	21	287710.072	0.0206

Table 5: Assigned transitions of the imidazole $^{13}\text{C}(2)$ isotopologue in the 12-15.5, 18-26, 75-110 and 260-295 GHz regions. For transitions in the 75-110 and 260-295 GHz regions, the F quantum numbers become redundant due to the absence of hyperfine structure, and the F values are set to the values of the J quantum numbers.

J'	K'_a	K'_c	F'_1	F'_2		J	K_a	K_c	F_1	F_2	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
1	0	1	0	1	←	0	0	0	1	1	14070.0789	0.0305
1	0	1	0	1	←	0	0	0	1	0	14070.0789	0.0305
1	0	1	0	1	←	0	0	0	1	2	14070.0789	0.0305
1	0	1	2	2	←	0	0	0	1	1	14070.3748	0.0332
1	0	1	2	2	←	0	0	0	1	2	14070.3748	0.0332
1	0	1	1	0	←	0	0	0	1	1	14070.653	-0.0023
1	0	1	1	1	←	0	0	0	1	0	14071.3924	0.0272
1	0	1	1	1	←	0	0	0	1	1	14071.3924	0.0272
1	0	1	1	1	←	0	0	0	1	2	14071.3924	0.0272
1	0	1	2	3	←	0	0	0	1	2	14071.5004	0.048
1	0	1	1	2	←	0	0	0	1	1	14071.7613	-0.0048
1	0	1	1	2	←	0	0	0	1	2	14071.7613	-0.0048
1	0	1	2	1	←	0	0	0	1	0	14073.3478	0.0055
1	0	1	2	1	←	0	0	0	1	2	14073.3478	0.0055
1	0	1	2	1	←	0	0	0	1	1	14073.3478	0.0055
2	2	1	2	1	←	2	0	2	1	1	14418.8944	-0.0111
2	2	1	1	2	←	2	0	2	3	2	14418.8944	-0.0378
2	2	1	3	4	←	2	0	2	3	4	14418.8944	0.0338
2	2	1	3	3	←	2	0	2	3	3	14420.8198	0.0261
2	0	2	1	2	←	1	1	1	1	2	23500.3434	0.0229
2	0	2	3	3	←	1	1	1	1	2	23500.3434	0.0307
2	0	2	3	3	←	1	1	1	2	2	23500.8036	0.0169
2	0	2	3	2	←	1	1	1	1	1	23501.2013	0.1021
2	0	2	1	2	←	1	1	1	2	1	23501.2013	-0.0326
2	0	2	3	4	←	1	1	1	2	3	23501.7353	0.0308
2	0	2	2	3	←	1	1	1	2	2	23502.3038	0.0285
2	1	2	1	1	←	1	1	1	1	0	23504.2919	0.027
2	1	2	1	2	←	1	1	1	1	2	23504.8634	0.0349
2	1	2	3	3	←	1	1	1	1	2	23504.8634	0.0268
2	1	2	3	3	←	1	1	1	2	2	23505.3259	0.0152
2	1	2	1	2	←	1	1	1	2	2	23505.3259	0.0233
2	1	2	1	2	←	1	1	1	2	1	23505.7003	-0.0417
2	1	2	3	2	←	1	1	1	1	1	23505.7003	0.1017
2	1	2	3	4	←	1	1	1	2	3	23506.2242	0.0271
2	1	2	2	2	←	1	1	1	1	2	23506.2242	0.0212
2	1	2	2	3	←	1	1	1	2	2	23506.793	0.0237
2	1	2	2	2	←	1	1	1	2	1	23507.1531	0.0365
2	1	2	2	1	←	1	1	1	2	1	23507.5156	0.0292
2	1	2	2	2	←	1	1	1	0	1	23507.794	0.0265

2	1	2	2	1	←	1	1	1	0	1	23508.165	0.0277
3	1	2	3	4	←	3	1	3	3	4	23582.7079	0.0301
3	1	2	4	5	←	3	1	3	3	4	23582.7079	0.0291
3	1	2	2	3	←	3	1	3	3	4	23582.7079	0.0288
3	1	2	4	5	←	3	1	3	4	5	23583.7439	0.0105
3	1	2	2	2	←	3	1	3	2	1	23583.7439	0.039
3	1	2	2	3	←	3	1	3	4	3	23583.7439	0.0485
3	1	2	3	4	←	3	1	3	4	5	23583.7439	0.0115
38	31	8	38	38	←	38	29	9	38	38	78682.6822	-0.0835
37	30	8	37	37	←	37	28	9	37	37	78836.1936	0.0017
36	29	8	36	36	←	36	27	9	36	36	78977.7069	-0.0871
34	26	8	34	34	←	34	26	9	34	34	79224.7415	0.0023
34	27	8	34	34	←	34	25	9	34	34	79227.8623	0.0125
33	26	8	33	33	←	33	24	9	33	33	79337.5218	0.0084
32	24	8	32	32	←	32	24	9	32	32	79436.5741	0.0154
32	25	8	32	32	←	32	23	9	32	32	79437.7478	0.0044
31	23	8	31	31	←	31	23	9	31	31	79528.4287	0.0081
31	24	8	31	31	←	31	22	9	31	31	79529.1426	0.0087
28	21	8	28	28	←	28	19	9	28	28	79755.8594	-0.0699
27	20	8	27	27	←	27	18	9	27	27	79817.4802	-0.0304
27	19	8	27	27	←	27	19	9	27	27	79817.4802	0.0471
25	17	8	25	25	←	25	17	9	25	25	79922.585	0.0149
25	18	8	25	25	←	25	16	9	25	25	79922.585	-0.0073
22	14	8	22	22	←	22	14	9	22	22	80041.59	0.0069
22	15	8	22	22	←	22	13	9	22	22	80041.59	0.0042
22	15	8	22	22	←	22	13	9	22	22	80041.5912	0.0053
22	14	8	22	22	←	22	14	9	22	22	80041.5912	0.0081
21	13	8	21	21	←	21	13	9	21	21	80072.6087	0.0619
21	14	8	21	21	←	21	12	9	21	21	80072.6087	0.0606
19	11	8	19	19	←	19	11	9	19	19	80123.5902	0.0191
19	12	8	19	19	←	19	10	9	19	19	80123.5902	0.0189
18	11	8	18	18	←	18	9	9	18	18	80144.2992	0.0168
18	10	8	18	18	←	18	10	9	18	18	80144.2992	0.0169
8	0	8	8	8	←	7	0	7	7	7	80197.3395	0.0382
8	1	8	8	8	←	7	1	7	7	7	80197.3395	0.0382
7	1	6	7	7	←	6	1	5	6	6	80202.4752	0.0045
7	2	6	7	7	←	6	2	5	6	6	80202.4752	0.0046
13	5	8	13	13	←	13	5	9	13	13	80211.24	-0.0014
13	6	8	13	13	←	13	4	9	13	13	80211.24	-0.0014
12	5	8	12	12	←	12	3	9	12	12	80219.0537	0.0088
12	4	8	12	12	←	12	4	9	12	12	80219.0537	0.0088
11	4	8	11	11	←	11	2	9	11	11	80225.4673	-0.0193
11	4	8	11	11	←	11	2	9	11	11	80225.4673	-0.0193
11	3	8	11	11	←	11	3	9	11	11	80225.4673	-0.0193
48	40	9	48	48	←	48	38	10	48	48	86833.8551	0.0023
46	38	9	46	46	←	46	36	10	46	46	87273.4309	0.0041

45	37	9	45	45	←	45	35	10	45	45	87472.8163	0.0214
43	35	9	43	43	←	43	33	10	43	43	87832.9352	-0.0189
42	34	9	42	42	←	42	32	10	42	42	87994.8718	0.0441
41	33	9	41	41	←	41	31	10	41	41	88145.3523	0.023
40	31	9	40	40	←	40	31	10	40	40	88282.7799	0.0215
40	32	9	40	40	←	40	30	10	40	40	88285.0418	-0.0009
39	30	9	39	39	←	39	30	10	39	39	88413.0954	0.0025
39	31	9	39	39	←	39	29	10	39	39	88414.5509	0.0048
38	29	9	38	38	←	38	29	10	38	38	88533.5097	0.0168
38	30	9	38	38	←	38	28	10	38	38	88534.4065	0.0009
36	27	9	36	36	←	36	27	10	36	36	88747.0741	0.0488
34	26	9	34	34	←	34	24	10	34	34	88928.0599	-0.03
33	25	9	33	33	←	33	23	10	33	33	89007.5264	-0.0343
33	24	9	33	33	←	33	24	10	33	33	89007.5264	0.0375
32	23	9	32	32	←	32	23	10	32	32	89080.3412	0.0111
32	24	9	32	32	←	32	22	10	32	32	89080.3412	-0.03
31	23	9	31	31	←	31	21	10	31	31	89146.9438	-0.0005
31	22	9	31	31	←	31	22	10	31	31	89146.9438	0.0226
30	22	9	30	30	←	30	20	10	30	30	89207.6849	0.0017
30	21	9	30	30	←	30	21	10	30	30	89207.6849	0.0144
29	21	9	29	29	←	29	19	10	29	29	89262.9732	0.001
29	20	9	29	29	←	29	20	10	29	29	89262.9732	0.0079
28	20	9	28	28	←	28	18	10	28	28	89313.1647	-0.0123
28	19	9	28	28	←	28	19	10	28	28	89313.1647	-0.0087
27	19	9	27	27	←	27	17	10	27	27	89358.6353	-0.0114
27	18	9	27	27	←	27	18	10	27	27	89358.6353	-0.0096
25	17	9	25	25	←	25	15	10	25	25	89436.6774	-0.0161
25	16	9	25	25	←	25	16	10	25	25	89436.6774	-0.0157
24	15	9	24	24	←	24	15	10	24	24	89469.8782	-0.0103
24	16	9	24	24	←	24	14	10	24	24	89469.8782	-0.0105
23	14	9	23	23	←	23	14	10	23	23	89499.6315	0.0457
23	15	9	23	23	←	23	13	10	23	23	89499.6315	0.0456
22	13	9	22	22	←	22	13	10	22	22	89526.0649	0.0069
22	14	9	22	22	←	22	12	10	22	22	89526.0649	0.0069
20	11	9	20	20	←	20	11	10	20	20	89570.3557	0.0025
20	12	9	20	20	←	20	10	10	20	20	89570.3557	0.0025
18	9	9	18	18	←	18	9	10	18	18	89604.7	0.0023
18	10	9	18	18	←	18	8	10	18	18	89604.7	0.0023
16	8	9	16	16	←	16	6	10	16	16	89630.8158	-0.0014
16	7	9	16	16	←	16	7	10	16	16	89630.8158	-0.0014
9	0	9	9	9	←	8	0	8	8	8	89631.7726	0.0305
9	1	9	9	9	←	8	1	8	8	8	89631.7726	0.0305
8	1	7	8	8	←	7	1	6	7	7	89636.8661	0.0328
8	2	7	8	8	←	7	2	6	7	7	89636.8661	0.0328
15	7	9	15	15	←	15	5	10	15	15	89641.2905	0.0103
15	6	9	15	15	←	15	6	10	15	15	89641.2905	0.0103

7	2	5	7	7	←	6	2	4	6	6	89642.7442	-0.0672
7	3	5	7	7	←	6	3	4	6	6	89642.7442	-0.0211
14	5	9	14	14	←	14	5	10	14	14	89650.2244	-0.0239
14	6	9	14	14	←	14	4	10	14	14	89650.2244	-0.0239
13	4	9	13	13	←	13	4	10	13	13	89657.8584	-0.027
13	5	9	13	13	←	13	3	10	13	13	89657.8584	-0.027
12	4	9	12	12	←	12	2	10	12	12	89664.3058	-0.0379
12	3	9	12	12	←	12	3	10	12	12	89664.3058	-0.0379
46	37	10	46	46	←	46	35	11	46	46	97296.4131	0.0024
45	35	10	45	45	←	45	35	11	45	45	97443.2894	0.0092
40	31	10	40	40	←	40	29	11	40	40	98047.9349	-0.0354
39	29	10	39	39	←	39	29	11	39	39	98144.7428	0.0174
39	30	10	39	39	←	39	28	11	39	39	98144.7428	-0.0426
38	28	10	38	38	←	38	28	11	38	38	98234.6172	0.0264
38	29	10	38	38	←	38	27	11	38	38	98234.6172	-0.0091
37	27	10	37	37	←	37	27	11	37	37	98317.903	0.0415
37	28	10	37	37	←	37	26	11	37	37	98317.903	0.0207
36	26	10	36	36	←	36	26	11	36	36	98394.9054	-0.0074
36	27	10	36	36	←	36	25	11	36	36	98394.9054	-0.0194
35	25	10	35	35	←	35	25	11	35	35	98466.1096	0.0072
35	26	10	35	35	←	35	24	11	35	35	98466.1096	0.0004
34	24	10	34	34	←	34	24	11	34	34	98531.7897	0.0191
34	25	10	34	34	←	34	23	11	34	34	98531.7897	0.0154
33	24	10	33	33	←	33	22	11	33	33	98592.2469	0.0021
33	23	10	33	33	←	33	23	11	33	33	98592.2469	0.0041
32	23	10	32	32	←	32	21	11	32	32	98647.8249	-0.0057
32	22	10	32	32	←	32	22	11	32	32	98647.8249	-0.0046
31	21	10	31	31	←	31	21	11	31	31	98698.8294	0.0016
31	22	10	31	31	←	31	20	11	31	31	98698.8294	0.001
29	20	10	29	29	←	29	18	11	29	29	98788.1818	-0.0007
29	19	10	29	29	←	29	19	11	29	29	98788.1818	-0.0005
28	19	10	28	28	←	28	17	11	28	28	98827.061	-0.0092
28	18	10	28	28	←	28	18	11	28	28	98827.061	-0.0091
27	18	10	27	27	←	27	16	11	27	27	98862.4268	-0.0067
27	17	10	27	27	←	27	17	11	27	27	98862.4268	-0.0067
25	15	10	25	25	←	25	15	11	25	25	98923.514	-0.014
25	16	10	25	25	←	25	14	11	25	25	98923.514	-0.014
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23	13	10	23	23	←	23	13	11	23	23	98973.2644	0.019
23	14	10	23	23	←	23	12	11	23	23	98973.2644	0.019
22	13	10	22	22	←	22	11	11	22	22	98994.2917	-0.0589
22	12	10	22	22	←	22	12	11	22	22	98994.2917	-0.0589
21	12	10	21	21	←	21	10	11	21	21	99013.2135	0.0049
21	11	10	21	21	←	21	11	11	21	21	99013.2135	0.0049
19	10	10	19	19	←	19	8	11	19	19	99044.8668	-0.0249

19	9	10	19	19	←	19	9	11	19	19	99044.8668	-0.0249
18	8	10	18	18	←	18	8	11	18	18	99058.0756	0.0255
18	9	10	18	18	←	18	7	11	18	18	99058.0756	0.0255
10	1	10	10	10	←	9	1	9	9	9	99066.1487	0.0417
10	0	10	10	10	←	9	0	9	9	9	99066.1487	0.0417
17	8	10	17	17	←	17	6	11	17	17	99069.6285	0.0013
17	7	10	17	17	←	17	7	11	17	17	99069.6285	0.0013
9	1	8	9	9	←	8	1	7	8	8	99071.1591	0.0156
9	2	8	9	9	←	8	2	7	8	8	99071.1591	0.0156
8	2	6	8	8	←	7	2	5	7	7	99076.6381	0.0028
8	3	6	8	8	←	7	3	5	7	7	99076.6381	0.0036
16	6	10	16	16	←	16	6	11	16	16	99079.7924	0.0244
16	7	10	16	16	←	16	5	11	16	16	99079.7924	0.0244
15	5	10	15	15	←	15	5	11	15	15	99088.657	0.0478
15	6	10	15	15	←	15	4	11	15	15	99088.657	0.0478
13	4	10	13	13	←	13	2	11	13	13	99102.8938	-0.0041
13	3	10	13	13	←	13	3	11	13	13	99102.8938	-0.0041
12	3	10	12	12	←	12	1	11	12	12	99108.5517	-0.0258
12	2	10	12	12	←	12	2	11	12	12	99108.5517	-0.0258
47	37	11	47	47	←	47	35	12	47	47	106997.6112	-0.0678
47	36	11	47	47	←	47	36	12	47	47	106997.6112	0.0541
45	34	11	45	45	←	45	34	12	45	45	107232.2052	0.0216
45	35	11	45	45	←	45	33	12	45	45	107232.2052	-0.0252
44	34	11	44	44	←	44	32	12	44	44	107338.5153	-0.0391
43	33	11	43	43	←	43	31	12	43	43	107438.1033	0.041
41	30	11	41	41	←	41	30	12	41	41	107618.0035	0.0193
41	31	11	41	41	←	41	29	12	41	41	107618.0035	0.0134
40	29	11	40	40	←	40	29	12	40	40	107699.0251	-0.0256
40	30	11	40	40	←	40	28	12	40	40	107699.0251	-0.0291
39	28	11	39	39	←	39	28	12	39	39	107774.5914	0.0014
39	29	11	39	39	←	39	27	12	39	39	107774.5914	-0.0004
38	27	11	38	38	←	38	27	12	38	38	107844.8766	-0.0147
38	28	11	38	38	←	38	26	12	38	38	107844.8766	-0.0158
37	27	11	37	37	←	37	25	12	37	37	107910.2278	-0.0052
37	26	11	37	37	←	37	26	12	37	37	107910.2278	-0.0046
36	26	11	36	36	←	36	24	12	36	36	107970.8666	-0.0136
36	25	11	36	36	←	36	25	12	36	36	107970.8666	-0.0132
34	24	11	34	34	←	34	22	12	34	34	108079.1122	0.0071
34	23	11	34	34	←	34	23	12	34	34	108079.1122	0.0072
33	23	11	33	33	←	33	21	12	33	33	108127.1613	-0.0022
33	22	11	33	33	←	33	22	12	33	33	108127.1613	-0.0022
32	21	11	32	32	←	32	21	12	32	32	108171.4761	-0.0147
32	22	11	32	32	←	32	20	12	32	32	108171.4761	-0.0147
31	21	11	31	31	←	31	19	12	31	31	108212.2762	-0.028
31	20	11	31	31	←	31	20	12	31	31	108212.2762	-0.028
30	19	11	30	30	←	30	19	12	30	30	108249.801	-0.0114

30	20	11	30	30	←	30	18	12	30	30	108249.801	-0.0114
29	18	11	29	29	←	29	18	12	29	29	108284.1967	-0.0191
29	19	11	29	29	←	29	17	12	29	29	108284.1967	-0.0191
28	17	11	28	28	←	28	17	12	28	28	108315.717	0.0103
28	18	11	28	28	←	28	16	12	28	28	108315.717	0.0103
26	16	11	26	26	←	26	14	12	26	26	108370.665	-0.0174
26	15	11	26	26	←	26	15	12	26	26	108370.665	-0.0174
24	14	11	24	24	←	24	12	12	24	24	108416.1044	-0.0231
24	13	11	24	24	←	24	13	12	24	24	108416.1044	-0.0231
23	13	11	23	23	←	23	11	12	23	23	108435.6794	0.0011
23	12	11	23	23	←	23	12	12	23	23	108435.6794	0.0011
22	11	11	22	22	←	22	11	12	22	22	108453.2402	-0.0747
22	12	11	22	22	←	22	10	12	22	22	108453.2402	-0.0747
21	10	11	21	21	←	21	10	12	21	21	108469.1667	-0.0131
21	11	11	21	21	←	21	9	12	21	21	108469.1667	-0.0131
20	9	11	20	20	←	20	9	12	20	20	108483.4366	0.0285
20	10	11	20	20	←	20	8	12	20	20	108483.4366	0.0285
19	8	11	19	19	←	19	8	12	19	19	108496.1445	0.0159
19	9	11	19	19	←	19	7	12	19	19	108496.1445	0.0159
11	0	11	11	11	←	10	0	10	10	10	108500.4259	0.0383
11	1	11	11	11	←	10	1	10	10	10	108500.4259	0.0383
10	2	9	10	10	←	9	2	8	9	9	108505.3942	0.0132
10	1	9	10	10	←	9	1	8	9	9	108505.3942	0.0132
18	8	11	18	18	←	18	6	12	18	18	108507.4693	0.0058
18	7	11	18	18	←	18	7	12	18	18	108507.4693	0.0058
16	5	11	16	16	←	16	5	12	16	16	108526.348	-0.0867
16	6	11	16	16	←	16	4	12	16	16	108526.348	-0.0867
15	5	11	15	15	←	15	3	12	15	15	108534.2784	-0.0055
15	4	11	15	15	←	15	4	12	15	15	108534.2784	-0.0055
13	3	11	13	13	←	13	1	12	13	13	108547.1749	-0.0205
13	2	11	13	13	←	13	2	12	13	13	108547.1749	-0.0205
7	4	3	7	7	←	6	4	2	6	6	108706.0093	-0.0713
24	3	21	24	24	←	23	4	20	23	23	259443.1459	-0.028
24	3	21	24	24	←	23	3	20	23	23	259443.1459	-0.028
24	4	21	24	24	←	23	4	20	23	23	259443.1459	-0.028
24	4	21	24	24	←	23	3	20	23	23	259443.1459	-0.028
23	5	19	23	23	←	22	5	18	22	22	259446.858	-0.0254
23	5	19	23	23	←	22	4	18	22	22	259446.858	-0.0254
23	4	19	23	23	←	22	5	18	22	22	259446.858	-0.0254
23	4	19	23	23	←	22	4	18	22	22	259446.858	-0.0254
21	7	15	21	21	←	20	6	14	20	20	259454.9605	0.0101
21	7	15	21	21	←	20	7	14	20	20	259454.9605	0.0101
21	6	15	21	21	←	20	6	14	20	20	259454.9605	0.0101
21	6	15	21	21	←	20	7	14	20	20	259454.9605	0.0101
20	8	13	20	20	←	19	7	12	19	19	259460.2233	0.0122
20	8	13	20	20	←	19	8	12	19	19	259460.2233	0.0122

20	7	13	20	20	←	19	8	12	19	19	259460.2233	0.0122
20	7	13	20	20	←	19	7	12	19	19	259460.2233	0.0122
19	9	11	19	19	←	18	8	10	18	18	259467.7626	0.0277
19	8	11	19	19	←	18	8	10	18	18	259467.7626	0.0277
19	9	11	19	19	←	18	9	10	18	18	259467.7626	0.0277
19	8	11	19	19	←	18	9	10	18	18	259467.7626	0.0277
18	10	9	18	18	←	17	9	8	17	17	259481.0102	0.0536
18	9	9	18	18	←	17	10	8	17	17	259481.0102	0.0536
18	10	9	18	18	←	17	10	8	17	17	259481.0121	0.0555
18	9	9	18	18	←	17	9	8	17	17	259481.0121	0.0555
31	5	27	31	31	←	31	3	28	31	31	259496.6182	-0.0054
31	4	27	31	31	←	31	4	28	31	31	259496.6182	-0.0054
17	10	7	17	17	←	16	10	6	16	16	259512.4613	0.0645
28	0	28	28	28	←	27	0	27	27	27	268862.1924	-0.0029
28	1	28	28	28	←	27	1	27	27	27	268862.1924	-0.0029
28	0	28	28	28	←	27	1	27	27	27	268862.1941	-0.0012
28	1	28	28	28	←	27	0	27	27	27	268862.1941	-0.0012
26	2	24	26	26	←	25	2	23	25	25	268870.7803	-0.0668
26	3	24	26	26	←	25	3	23	25	25	268870.7803	-0.0668
26	2	24	26	26	←	25	3	23	25	25	268870.7824	-0.0647
26	3	24	26	26	←	25	2	23	25	25	268870.7824	-0.0647
25	4	22	25	25	←	24	4	21	24	24	268874.5219	-0.0796
25	3	22	25	25	←	24	3	21	24	24	268874.5219	-0.0796
25	3	22	25	25	←	24	4	21	24	24	268874.5239	-0.0776
25	4	22	25	25	←	24	3	21	24	24	268874.5239	-0.0776
24	5	20	24	24	←	23	5	19	23	23	268878.1627	-0.0385
24	4	20	24	24	←	23	4	19	23	23	268878.1627	-0.0385
24	5	20	24	24	←	23	4	19	23	23	268878.1651	-0.0361
24	4	20	24	24	←	23	5	19	23	23	268878.1651	-0.0361
23	6	18	23	23	←	22	6	17	22	22	268881.8141	-0.0431
23	5	18	23	23	←	22	5	17	22	22	268881.8141	-0.0431
23	5	18	23	23	←	22	6	17	22	22	268881.8164	-0.0408
23	6	18	23	23	←	22	5	17	22	22	268881.8164	-0.0408
22	7	16	22	22	←	21	7	15	21	21	268885.9086	0.0492
22	6	16	22	22	←	21	6	15	21	21	268885.9086	0.0492
22	6	16	22	22	←	21	7	15	21	21	268885.9105	0.0511
22	7	16	22	22	←	21	6	15	21	21	268885.9105	0.0511
21	7	14	21	21	←	20	7	13	20	20	268890.7196	0.0385
21	8	14	21	21	←	20	8	13	20	20	268890.7196	0.0385
21	8	14	21	21	←	20	7	13	20	20	268890.7201	0.039
21	7	14	21	21	←	20	8	13	20	20	268890.7201	0.039
19	9	10	19	19	←	18	9	9	18	18	268907.9847	0.0558
19	10	10	19	19	←	18	10	9	18	18	268907.9847	0.0558
19	10	10	19	19	←	18	9	9	18	18	268907.9866	0.0576
19	9	10	19	19	←	18	10	9	18	18	268907.9866	0.0576
18	10	8	18	18	←	17	10	7	17	17	268929.9401	0.0002

18	11	8	18	18	←	17	11	7	17	17	268929.9401	0.0035
18	10	8	18	18	←	17	11	7	17	17	268929.9421	0.0056
18	11	8	18	18	←	17	10	7	17	17	268929.9421	0.0021
17	12	6	17	17	←	16	12	5	16	16	268993.0711	-0.0391
36	8	29	36	36	←	36	7	30	36	36	278290.291	0.0677
36	8	29	36	36	←	36	6	30	36	36	278290.291	0.0677
36	7	29	36	36	←	36	7	30	36	36	278290.291	0.0677
36	7	29	36	36	←	36	6	30	36	36	278290.291	0.0677
29	0	29	29	29	←	28	0	28	28	28	278293.5375	0.0216
29	1	29	29	29	←	28	1	28	28	28	278293.5375	0.0216
29	0	29	29	29	←	28	1	28	28	28	278293.5377	0.0218
29	1	29	29	29	←	28	0	28	28	28	278293.5377	0.0218
28	2	27	28	28	←	27	2	26	27	27	278298.0836	0.0131
28	1	27	28	28	←	27	1	26	27	27	278298.0836	0.0131
28	1	27	28	28	←	27	2	26	27	27	278298.0859	0.0154
28	2	27	28	28	←	27	1	26	27	27	278298.0859	0.0154
27	3	25	27	27	←	26	3	24	26	26	278302.075	-0.0366
27	2	25	27	27	←	26	2	24	26	26	278302.075	-0.0366
27	2	25	27	27	←	26	3	24	26	26	278302.0766	-0.035
27	3	25	27	27	←	26	2	24	26	26	278302.0766	-0.035
26	3	23	26	26	←	25	3	22	25	25	278305.7976	0.0033
26	4	23	26	26	←	25	4	22	25	25	278305.7976	0.0033
26	4	23	26	26	←	25	3	22	25	25	278305.8004	0.006
26	3	23	26	26	←	25	4	22	25	25	278305.8004	0.006
24	6	19	24	24	←	23	6	18	23	23	278312.7481	-0.0439
24	5	19	24	24	←	23	5	18	23	23	278312.7481	-0.0439
24	6	19	24	24	←	23	5	18	23	23	278312.7505	-0.0415
24	5	19	24	24	←	23	6	18	23	23	278312.7505	-0.0415
23	7	17	23	23	←	22	7	16	22	22	278316.5321	-0.0361
23	6	17	23	23	←	22	6	16	22	22	278316.5321	-0.0361
23	7	17	23	23	←	22	6	16	22	22	278316.5346	-0.0336
23	6	17	23	23	←	22	7	16	22	22	278316.5346	-0.0336
20	10	11	20	20	←	19	10	10	19	19	278335.7499	-0.0311
20	9	11	20	20	←	19	9	10	19	19	278335.7499	-0.0311
20	10	11	20	20	←	19	9	10	19	19	278335.7515	-0.0294
20	9	11	20	20	←	19	10	10	19	19	278335.7515	-0.0294
20	10	11	20	20	←	19	10	10	19	19	278335.7515	-0.0294
19	10	9	19	19	←	18	11	8	18	18	278352.2776	-0.0258
19	11	9	19	19	←	18	10	8	18	18	278352.2776	-0.0259
19	11	9	19	19	←	18	11	8	18	18	278352.2776	-0.0258
19	10	9	19	19	←	18	10	8	18	18	278352.2776	-0.0259
18	11	7	18	18	←	17	11	6	17	17	278393.1646	-0.0081
18	12	7	18	18	←	17	11	6	17	17	278393.165	-0.0155
17	13	5	17	17	←	16	13	4	16	16	278495.5004	0.0934
30	0	30	30	30	←	29	1	29	29	29	287724.6711	0.0858
30	1	30	30	30	←	29	0	29	29	29	287724.6711	0.0858

30	1	30	30	30	←	29	1	29	29	29	287724.6723	0.087
30	0	30	30	30	←	29	0	29	29	29	287724.6723	0.087
29	2	28	29	29	←	28	1	27	28	28	287729.1918	0.0634
29	1	28	29	29	←	28	2	27	28	28	287729.1918	0.0634
29	2	28	29	29	←	28	2	27	28	28	287729.1931	0.0647
29	1	28	29	29	←	28	1	27	28	28	287729.1931	0.0647
28	2	26	28	28	←	27	3	25	27	27	287733.1846	0.0549
28	3	26	28	28	←	27	2	25	27	27	287733.1846	0.0549
28	3	26	28	28	←	27	3	25	27	27	287733.1863	0.0565
28	2	26	28	28	←	27	2	25	27	27	287733.1863	0.0565
26	4	22	26	26	←	25	5	21	25	25	287740.0648	-0.069
26	5	22	26	26	←	25	4	21	25	25	287740.0648	-0.069
26	5	22	26	26	←	25	5	21	25	25	287740.0662	-0.0676
26	4	22	26	26	←	25	4	21	25	25	287740.0662	-0.0676
24	7	18	24	24	←	23	6	17	23	23	287747.0881	0.0279
24	6	18	24	24	←	23	7	17	23	23	287747.0881	0.0279
24	6	18	24	24	←	23	6	17	23	23	287747.0912	0.031
24	7	18	24	24	←	23	6	17	23	23	287747.0912	0.031
23	8	16	23	23	←	22	7	15	22	22	287751.1342	-0.0483
23	7	16	23	23	←	22	8	15	22	22	287751.1342	-0.0483
23	8	16	23	23	←	22	8	15	22	22	287751.1358	-0.0467
23	7	16	23	23	←	22	7	15	22	22	287751.1358	-0.0467
22	8	14	22	22	←	21	9	13	21	21	287756.4476	-0.0046
22	9	14	22	22	←	21	8	13	21	21	287756.4476	-0.0046
22	8	14	22	22	←	21	8	13	21	21	287756.4479	-0.0043
22	9	14	22	22	←	21	9	13	21	21	287756.4479	-0.0043
21	9	12	21	21	←	20	10	11	20	20	287764.0628	-0.0225
21	10	12	21	21	←	20	10	11	20	20	287764.0628	-0.0225
21	10	12	21	21	←	20	9	11	20	20	287764.0628	-0.0225
21	9	12	21	21	←	20	9	11	20	20	287764.0628	-0.0225
21	10	12	21	21	←	20	10	11	20	20	287764.065	-0.0203
21	9	12	21	21	←	20	9	11	20	20	287764.065	-0.0203
20	11	10	20	20	←	19	10	9	19	19	287777.0954	-0.0273
20	10	10	20	20	←	19	11	9	19	19	287777.0954	-0.0273
20	11	10	20	20	←	19	11	9	19	19	287777.0958	-0.0269
20	10	10	20	20	←	19	10	9	19	19	287777.0958	-0.0269
19	12	8	19	19	←	18	11	7	18	18	287805.0855	-0.0652
19	11	8	19	19	←	18	12	7	18	18	287805.0855	-0.0573

Table 6: Assigned transitions of the imidazole $^{15}\text{N}(3)$ isotopologue in the 2-8, 12-15.5, 18-26, 75-110 and 260-295 GHz regions. For transitions in the 75-110 and 260-295 GHz regions, the F quantum number becomes redundant due to the absence of hyperfine structure, and the F value is set to the value of the J quantum number.

J'	K'_a	K'_c	F'		J	K_a	K_c	F	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
1	1	0	2	←	1	1	1	1	4427.0575	-0.0056
1	1	0	1	←	1	1	1	0	4427.2579	0.0003
1	1	0	2	←	1	1	1	2	4427.448	-0.004
1	0	1	0	←	0	0	0	1	13843.591	0.0173
1	0	1	2	←	0	0	0	1	13844.1662	0.0093
1	0	1	1	←	0	0	0	1	13844.543	-0.0027
1	1	1	2	←	0	0	0	1	14429.9446	0.0048
2	0	2	1	←	1	1	1	1	23205.842	0.013
2	0	2	3	←	1	1	1	2	23206.7228	0.0447
2	0	2	3	←	1	1	1	2	23206.7228	0.0447
2	0	2	1	←	1	1	1	0	23206.7228	-0.0782
2	0	2	2	←	1	1	1	1	23207.1436	0.0259
2	1	2	1	←	1	1	1	1	23260.226	0.0346
2	1	2	3	←	1	1	1	2	23261.0768	0.0336
2	1	2	3	←	1	1	1	2	23261.0768	0.0337
2	1	2	1	←	1	1	1	0	23261.0768	-0.0866
2	1	2	2	←	1	1	1	1	23261.5083	0.0207
2	1	2	2	←	1	1	1	2	23261.894	0.0176
3	1	2	3	←	3	1	3	3	23363.5186	-0.0334
3	1	2	4	←	3	1	3	4	23364.6484	0.0056
3	1	2	2	←	3	1	3	2	23365.0677	0.0432
3	2	2	4	←	3	0	3	3	23635.5156	-0.0031
3	2	2	4	←	3	0	3	4	23636.6033	0.0061
3	2	2	2	←	3	0	3	2	23636.9872	0.0126
2	0	2	1	←	1	0	1	1	23791.6443	0.0324
2	0	2	3	←	1	0	1	2	23792.4796	0.0186
2	0	2	1	←	1	0	1	0	23792.4796	-0.1043
2	0	2	2	←	1	0	1	1	23792.9175	0.017
2	0	2	2	←	1	0	1	2	23793.2947	0.0053
2	1	2	3	←	1	0	1	2	23846.8476	0.0216
2	1	2	2	←	1	0	1	1	23847.2658	-0.0045
25	17	8	25	←	25	17	9	25	76361.4223	0.0547
24	16	8	24	←	24	16	9	24	77021.5332	-0.0162
24	17	8	24	←	24	15	9	24	77231.3822	-0.0341
23	15	8	23	←	23	15	9	23	77561.0589	-0.0418
23	16	8	23	←	23	14	9	23	77669.3009	-0.0133
22	14	8	22	←	22	14	9	22	78008.2678	-0.0023
22	15	8	22	←	22	13	9	22	78061.9961	-0.0162
20	12	8	20	←	20	12	9	20	78697.9789	-0.0044

20	13	8	20	←	20	11	9	20	78709.6841	-0.0028
19	11	8	19	←	19	11	9	19	78964.2564	0.0332
19	12	8	19	←	19	10	9	19	78969.2948	-0.0205
18	11	8	18	←	18	9	9	18	79190.9358	0.0084
15	8	8	15	←	15	6	9	15	79666.6085	0.0407
15	7	8	15	←	15	7	9	15	79666.6085	0.14
14	6	8	14	←	14	6	9	14	79774.1563	0.0666
14	7	8	14	←	14	5	9	14	79774.1563	0.0363
13	5	8	13	←	13	5	9	13	79861.5595	0.0282
13	6	8	13	←	13	4	9	13	79861.5595	0.0199
11	4	8	11	←	11	2	9	11	79986.9044	-0.032
11	3	8	11	←	11	3	9	11	79986.9044	-0.0316
11	4	8	11	←	11	2	9	11	79986.9044	-0.032
11	3	8	11	←	11	3	9	11	79986.9044	-0.0316
10	2	8	10	←	10	2	9	10	80029.8069	0.0389
10	3	8	10	←	10	1	9	10	80029.8069	0.0388
8	0	8	8	←	7	0	7	7	80046.0739	0.0618
8	1	8	8	←	7	1	7	7	80046.0739	0.0618
7	2	6	7	←	6	2	5	6	80052.9628	0.0099
7	1	6	7	←	6	1	5	6	80052.9628	-0.0599
31	23	9	31	←	31	21	10	31	83955.2201	-0.0093
30	22	9	30	←	30	20	10	30	84553.74	0.032
29	20	9	29	←	29	20	10	29	84745.7314	-0.0033
28	19	9	28	←	28	19	10	28	85483.0666	-0.0088
28	20	9	28	←	28	18	10	28	85700.4873	-0.0184
27	19	9	27	←	27	17	10	27	86215.5441	0.0175
26	18	9	26	←	26	16	10	26	86682.4968	0.0171
25	16	9	25	←	25	16	10	25	87070.6805	-0.004
25	17	9	25	←	25	15	10	25	87100.3692	-0.0121
24	15	9	24	←	24	15	10	24	87456.4764	-0.0139
24	16	9	24	←	24	14	10	24	87470.787	0.0049
23	14	9	23	←	23	14	10	23	87789.96	-0.0278
23	15	9	23	←	23	13	10	23	87796.6055	-0.0043
22	13	9	22	←	22	13	10	22	88078.4153	-0.067
22	14	9	22	←	22	12	10	22	88081.4208	-0.0064
21	12	9	21	←	21	12	10	21	88327.7118	-0.0172
21	13	9	21	←	21	11	10	21	88328.966	-0.0151
18	9	9	18	←	18	9	10	18	88883.825	0.0474
18	10	9	18	←	18	8	10	18	88883.825	-0.0223
16	7	9	16	←	16	7	10	16	89129.0589	0.0393
16	8	9	16	←	16	6	10	16	89129.0589	0.032
15	7	9	15	←	15	5	10	15	89222.4669	0.0312
15	6	9	15	←	15	6	10	15	89222.4669	0.0333
14	5	9	14	←	14	5	10	14	89299.5225	-0.0045
14	6	9	14	←	14	4	10	14	89299.5225	-0.005
12	3	9	12	←	12	3	10	12	89412.9858	-0.0294

12	4	9	12	←	12	2	10	12	89412.9858	-0.0294
11	2	9	11	←	11	2	10	11	89453.073	-0.035
11	3	9	11	←	11	1	10	11	89453.073	-0.035
9	0	9	9	←	8	0	8	8	89462.6264	0.0104
9	1	9	9	←	8	1	8	8	89462.6264	0.0104
8	1	7	8	←	7	1	6	7	89468.9199	0.0121
8	2	7	8	←	7	2	6	7	89468.9199	0.0155
34	25	10	34	←	34	23	11	34	92784.9194	-0.0379
33	23	10	33	←	33	23	11	33	93064.0451	-0.0417
33	24	10	33	←	33	22	11	33	93454.4302	-0.0162
32	23	10	32	←	32	21	11	32	94088.1066	0.0031
31	22	10	31	←	31	20	11	31	94675.6064	0.0162
30	20	10	30	←	30	20	11	30	95149.6794	0.0412
30	21	10	30	←	30	19	11	30	95212.4772	-0.0102
29	19	10	29	←	29	19	11	29	95665.7999	0.0068
29	20	10	29	←	29	18	11	29	95698.1467	-0.0165
28	18	10	28	←	28	18	11	28	96118.0527	-0.0127
28	19	10	28	←	28	17	11	28	96134.2612	0.0093
27	17	10	27	←	27	17	11	27	96515.7892	0.0126
27	18	10	27	←	27	16	11	27	96523.6459	0.0252
25	15	10	25	←	25	15	11	25	97174.4281	-0.0212
25	16	10	25	←	25	14	11	25	97176.1139	0.002
24	14	10	24	←	24	14	11	24	97445.6218	-0.0305
24	15	10	24	←	24	13	11	24	97446.3669	-0.0087
22	12	10	22	←	22	12	11	22	97891.6262	0.0522
22	13	10	22	←	22	11	11	22	97891.6262	-0.0679
21	11	10	21	←	21	11	11	21	98072.7309	-0.0002
21	12	10	21	←	21	10	11	21	98072.7309	-0.0456
20	10	10	20	←	20	10	11	20	98229.7494	-0.0041
20	11	10	20	←	20	9	11	20	98229.7494	-0.0203
19	9	10	19	←	19	9	11	19	98365.0735	-0.0448
19	10	10	19	←	19	8	11	19	98365.0735	-0.0502
18	9	10	18	←	18	7	11	18	98481.1124	0.0185
18	8	10	18	←	18	8	11	18	98481.1124	0.0202
16	6	10	16	←	16	6	11	16	98663.094	0.0575
16	7	10	16	←	16	5	11	16	98663.094	0.0574
15	5	10	15	←	15	5	11	15	98732.7446	0.0445
15	6	10	15	←	15	4	11	15	98732.7446	0.0445
12	2	10	12	←	12	2	11	12	98875.7729	0.0141
12	3	10	12	←	12	1	11	12	98875.7729	0.0141
9	1	8	9	←	8	1	7	8	98885.0577	0.0146
9	2	8	9	←	8	2	7	8	98885.0577	0.0147
34	23	11	34	←	34	23	12	34	103600.0626	-0.028
34	24	11	34	←	34	22	12	34	103664.1145	-0.0001
33	22	11	33	←	33	22	12	33	104179.9924	0.0618
33	23	11	33	←	33	21	12	33	104213.747	0.0014

32	21	11	32	←	32	21	12	32	104694.6867	-0.0077
32	22	11	32	←	32	20	12	32	104712.1163	0.0121
31	20	11	31	←	31	20	12	31	105153.3807	0.052
31	21	11	31	←	31	19	12	31	105162.0756	0.0201
30	19	11	30	←	30	19	12	30	105562.7277	0.0201
30	20	11	30	←	30	18	12	30	105567.0181	0.0576
29	18	11	29	←	29	18	12	29	105928.34	0.0355
28	17	11	28	←	28	17	12	28	106254.6371	0.0072
28	18	11	28	←	28	16	12	28	106255.5639	0.0122
26	15	11	26	←	26	15	12	26	106804.3737	0.0785
26	16	11	26	←	26	14	12	26	106804.3737	-0.0957
25	14	11	25	←	25	14	12	25	107033.9709	0.0404
25	15	11	25	←	25	13	12	25	107033.9709	-0.031
24	14	11	24	←	24	12	12	24	107237.0188	-0.0931
24	13	11	24	←	24	13	12	24	107237.0188	-0.065
23	13	11	23	←	23	11	12	23	107416.1488	-0.0379
23	12	11	23	←	23	12	12	23	107416.1488	-0.0273
21	11	11	21	←	21	9	12	21	107710.8426	-0.0287
21	10	11	21	←	21	10	12	21	107710.8426	-0.0274
20	9	11	20	←	20	9	12	20	107830.3575	-0.0418
20	10	11	20	←	20	8	12	20	107830.3575	-0.0422
19	9	11	19	←	19	7	12	19	107933.7375	-0.0239
19	8	11	19	←	19	8	12	19	107933.7375	-0.0238
18	7	11	18	←	18	6	12	18	108022.5573	-0.023
18	7	11	18	←	18	7	12	18	108022.5573	-0.023
16	5	11	16	←	16	5	12	16	108162.5755	0.0476
16	6	11	16	←	16	4	12	16	108162.5755	0.0476
14	4	11	14	←	14	2	12	14	108261.135	0.0253
14	3	11	14	←	14	3	12	14	108261.135	0.0253
11	0	11	11	←	10	0	10	10	108295.6385	0.0297
11	1	11	11	←	10	1	10	10	108295.6385	0.0297
13	2	11	13	←	13	2	12	13	108297.8865	0.0114
13	3	11	13	←	13	1	12	13	108297.8865	0.0114
10	1	9	10	←	9	1	8	9	108301.194	-0.0482
10	2	9	10	←	9	2	8	9	108301.194	-0.0482
9	3	7	9	←	8	3	6	8	108310.751	-0.0305
9	2	7	9	←	8	2	6	8	108310.751	-0.054
28	1	28	28	←	27	0	27	27	268354.5343	-0.0106
28	0	28	28	←	27	0	27	27	268354.5343	-0.0106
28	1	28	28	←	27	1	27	27	268354.5343	-0.0106
28	0	28	28	←	27	1	27	27	268354.5343	-0.0106
27	1	26	27	←	26	1	25	26	268359.1036	-0.0356
27	2	26	27	←	26	1	25	26	268359.1036	-0.0356
27	2	26	27	←	26	2	25	26	268359.1036	-0.0356
27	1	26	27	←	26	2	25	26	268359.1036	-0.0356
26	2	24	26	←	25	3	23	25	268363.3518	-0.0778

26	2	24	26	←	25	2	23	25	268363.3518	-0.0778
26	3	24	26	←	25	2	23	25	268363.3518	-0.0778
26	3	24	26	←	25	3	23	25	268363.3518	-0.0778
25	4	22	25	←	24	4	21	24	268367.7273	-0.0767
25	4	22	25	←	24	3	21	24	268367.7273	-0.0767
25	3	22	25	←	24	3	21	24	268367.7273	-0.0767
25	3	22	25	←	24	4	21	24	268367.7273	-0.0767
24	4	20	24	←	23	5	19	23	268372.8151	-0.0595
24	5	20	24	←	23	4	19	23	268372.8151	-0.0595
24	5	20	24	←	23	5	19	23	268372.8151	-0.0595
24	4	20	24	←	23	4	19	23	268372.8151	-0.0595
22	6	16	22	←	21	7	15	21	268390.3029	-0.0453
22	6	16	22	←	21	6	15	21	268390.3029	-0.0453
22	7	16	22	←	21	7	15	21	268390.3029	-0.0453
22	7	16	22	←	21	6	15	21	268390.3029	-0.0453
20	8	12	20	←	19	9	11	19	268446.1333	-0.0258
20	9	12	20	←	19	8	11	19	268446.1333	-0.0259
20	9	12	20	←	19	9	11	19	268446.1333	-0.0258
20	8	12	20	←	19	8	11	19	268446.1333	-0.0259
29	0	29	29	←	28	0	28	28	277768.0315	-0.0185
29	1	29	29	←	28	0	28	28	277768.0315	-0.0185
29	0	29	29	←	28	1	28	28	277768.0315	-0.0185
29	1	29	29	←	28	1	28	28	277768.0315	-0.0185
28	2	27	28	←	27	2	26	27	277772.675	0.053
28	1	27	28	←	27	2	26	27	277772.675	0.053
28	2	27	28	←	27	1	26	27	277772.675	0.053
28	1	27	28	←	27	1	26	27	277772.675	0.053
27	2	25	27	←	26	2	24	26	277776.8519	0.0045
27	3	25	27	←	26	2	24	26	277776.8519	0.0045
27	2	25	27	←	26	3	24	26	277776.8519	0.0045
27	3	25	27	←	26	3	24	26	277776.8519	0.0045
26	3	23	26	←	25	3	22	25	277781.1428	0.0561
26	4	23	26	←	25	4	22	25	277781.1428	0.0561
26	4	23	26	←	25	3	22	25	277781.1428	0.0561
26	3	23	26	←	25	4	22	25	277781.1428	0.0561
25	4	21	25	←	24	4	20	24	277785.9152	0.0252
25	5	21	25	←	24	4	20	24	277785.9152	0.0252
25	4	21	25	←	24	5	20	24	277785.9152	0.0252
25	5	21	25	←	24	5	20	24	277785.9152	0.0252
22	7	15	22	←	21	7	14	21	277817.6168	-0.084
22	8	15	22	←	21	8	14	21	277817.6168	-0.084
22	8	15	22	←	21	7	14	21	277817.6168	-0.084
22	7	15	22	←	21	8	14	21	277817.6168	-0.084
27	4	24	27	←	26	4	23	26	287194.179	0.0434
27	3	24	27	←	26	4	23	26	287194.179	0.0434
27	4	24	27	←	26	3	23	26	287194.179	0.0434

27	3	24	27	←	26	3	23	26	287194.179	0.0434
26	5	22	26	←	25	5	21	25	287198.7976	0.099
26	4	22	26	←	25	4	21	25	287198.7976	0.099
26	5	22	26	←	25	4	21	25	287198.7976	0.099
26	4	22	26	←	25	5	21	25	287198.7976	0.099
25	5	20	25	←	24	5	19	24	287204.5189	0.002
25	6	20	25	←	24	6	19	24	287204.5189	0.002
25	6	20	25	←	24	5	19	24	287204.5189	0.002
25	5	20	25	←	24	6	19	24	287204.5189	0.002
24	7	18	24	←	23	7	17	23	287213.0775	0.062
24	6	18	24	←	23	7	17	23	287213.0775	0.062
24	7	18	24	←	23	6	17	23	287213.0775	0.062
24	6	18	24	←	23	6	17	23	287213.0775	0.062
23	8	16	23	←	22	7	15	22	287226.982	0.0451
23	7	16	23	←	22	8	15	22	287226.982	0.0451
23	7	16	23	←	22	7	15	22	287226.982	0.0451
23	8	16	23	←	22	8	15	22	287226.982	0.0451
20	11	10	20	←	19	10	9	19	287414.43	-0.1421
20	10	10	20	←	19	11	9	19	287414.43	0.0624
20	11	10	20	←	19	11	9	19	287414.43	0.0465
20	10	10	20	←	19	10	9	19	287414.43	-0.1262

Table 7: Assigned transitions of the imidazole $^{13}\text{C}(4)$ isotopologue in the 2-8, 12-15.5, 18-26, 75-110 and 260-295 GHz regions. For transitions in the 75-110 and 260-295 GHz regions, the F quantum numbers become redundant due to the absence of hyperfine structure, and the F values are set to the values of the J quantum numbers.

J'	K'_a	K'_c	F'_1	F'_2		J	K_a	K_c	F_1	F_2	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
1	1	0	1	2	←	1	1	1	2	2	4572.6843	-0.0115
1	1	0	2	3	←	1	1	1	2	3	4573.4519	0.0062
1	1	0	2	3	←	1	1	1	2	3	4573.4519	0.0062
1	1	0	2	2	←	1	1	1	1	1	4573.6444	-0.0039
1	1	0	0	1	←	1	1	1	1	2	4574.474	0.0104
1	1	0	0	1	←	1	1	1	1	2	4574.474	0.0104
2	1	1	2	3	←	2	1	2	2	3	13718.9395	-0.0022
2	1	1	3	4	←	2	1	2	3	4	13720.141	-0.0112
2	1	1	3	3	←	2	1	2	3	3	13720.6963	-0.0423
1	0	1	0	1	←	0	0	0	1	2	13997.4015	-0.043
1	0	1	2	2	←	0	0	0	1	2	13997.7957	0.0243
1	0	1	2	2	←	0	0	0	1	1	13997.7957	0.0243
1	0	1	1	0	←	0	0	0	1	1	13998.0816	-0.0057
1	0	1	2	1	←	0	0	0	1	1	13998.4917	0.0492
1	0	1	2	3	←	0	0	0	1	2	13998.4917	-0.0075
1	0	1	2	1	←	0	0	0	1	0	13998.4917	0.0493
1	0	1	2	1	←	0	0	0	1	2	13998.4917	0.0492
1	0	1	1	2	←	0	0	0	1	2	13998.8289	0.0137
1	0	1	1	2	←	0	0	0	1	1	13998.8289	0.0137
1	0	1	1	1	←	0	0	0	1	1	13999.8341	0.0174
1	0	1	1	1	←	0	0	0	1	2	13999.8341	0.0174
1	1	1	0	1	←	0	0	0	1	2	14285.7427	0.0519
1	1	1	2	3	←	0	0	0	1	2	14286.2602	-0.0028
1	1	1	2	1	←	0	0	0	1	1	14286.2602	0.0581
1	1	1	1	2	←	0	0	0	1	2	14286.6997	0.0167
2	2	1	2	3	←	2	0	2	2	3	14595.6744	-0.0075
2	2	1	3	4	←	2	0	2	3	4	14596.8146	-0.0263
2	2	1	3	3	←	2	0	2	3	3	14598.352	-0.0275
2	0	2	3	4	←	1	1	1	2	3	23410.4046	0.0148
2	0	2	2	3	←	1	1	1	1	2	23410.8037	0.0555
2	1	2	1	2	←	1	1	1	1	2	23422.5025	0.0494
2	1	2	3	3	←	1	1	1	2	2	23422.7991	0.0128
2	1	2	3	4	←	1	1	1	2	3	23423.5682	0.0158
2	1	2	3	4	←	1	1	1	2	3	23423.5682	0.0158
2	1	2	2	3	←	1	1	1	1	2	23423.9737	0.061
3	2	2	3	3	←	3	0	3	4	3	23594.8836	0.048
3	2	2	3	3	←	3	0	3	2	3	23595.4525	0.0186
3	2	2	4	4	←	3	0	3	4	4	23595.7711	-0.0192
2	0	2	1	0	←	1	0	1	1	1	23696.8137	0.0117

2	0	2	1	2	←	1	0	1	1	2	23697.1605	0.0163
2	0	2	3	3	←	1	0	1	1	2	23697.1605	0.0396
2	0	2	2	2	←	1	0	1	1	1	23697.5563	0.0129
2	0	2	3	3	←	1	0	1	2	2	23698.1922	0.0275
2	0	2	3	4	←	1	0	1	2	3	23698.1922	0.0386
2	0	2	2	3	←	1	0	1	1	2	23698.6211	0.0052
2	0	2	2	3	←	1	0	1	2	3	23698.9656	0.0337
2	0	2	2	2	←	1	0	1	2	2	23699.6259	0.0373
42	35	8	42	42	←	42	33	9	42	42	74894.1059	0.049
38	30	8	38	38	←	38	30	9	38	38	74943.583	0.009
41	34	8	41	41	←	41	32	9	41	41	75081.6283	-0.0156
40	33	8	40	40	←	40	31	9	40	40	75345.3063	0.0016
37	29	8	37	37	←	37	29	9	37	37	75636.6418	0.0107
38	31	8	38	38	←	38	29	9	38	38	75997.0613	-0.0119
37	30	8	37	37	←	37	28	9	37	37	76347.3265	0.0267
36	29	8	36	36	←	36	27	9	36	36	76696.1736	0.0085
35	27	8	35	35	←	35	27	9	35	35	76726.5041	-0.0007
35	28	8	35	35	←	35	26	9	35	35	77035.0377	0.0041
34	27	8	34	34	←	34	25	9	34	34	77358.0394	-0.0161
33	25	8	33	33	←	33	25	9	33	33	77536.052	-0.0148
33	26	8	33	33	←	33	24	9	33	33	77661.5449	-0.002
32	25	8	32	32	←	32	23	9	32	32	77943.4522	-0.0099
31	23	8	31	31	←	31	23	9	31	31	78155.3777	-0.0007
31	24	8	31	31	←	31	22	9	31	31	78202.9625	0.0035
30	22	8	30	30	←	30	22	9	30	30	78411.4972	-0.0694
30	23	8	30	30	←	30	21	9	30	30	78439.9994	-0.0485
29	21	8	29	29	←	29	21	9	29	29	78638.6427	0.0299
28	21	8	28	28	←	28	19	9	28	28	78849.7337	-0.0055
27	19	8	27	27	←	27	19	9	27	27	79019.0338	-0.0758
27	20	8	27	27	←	27	18	9	27	27	79024.526	0.0333
26	18	8	26	26	←	26	18	9	26	26	79177.9563	0.023
26	19	8	26	26	←	26	17	9	26	26	79180.8558	-0.0252
25	17	8	25	25	←	25	17	9	25	25	79318.6841	0.01
25	18	8	25	25	←	25	16	9	25	25	79320.2626	0.0161
24	16	8	24	24	←	24	16	9	24	24	79443.1716	0.0646
23	16	8	23	23	←	23	14	9	23	23	79552.9716	-0.2324
23	15	8	23	23	←	23	15	9	23	23	79552.9716	0.1774
22	14	8	22	22	←	22	14	9	22	22	79649.1706	0.0382
21	14	8	21	21	←	21	12	9	21	21	79733.4185	-0.0617
21	13	8	21	21	←	21	13	9	21	21	79733.4185	0.0315
20	13	8	20	20	←	20	11	9	20	20	79806.7134	-0.0441
20	12	8	20	20	←	20	12	9	20	20	79806.7134	-0.0021
18	10	8	18	18	←	18	10	9	18	18	79924.8096	0.0267
18	11	8	18	18	←	18	9	9	18	18	79924.8096	0.0194
17	10	8	17	17	←	17	8	9	17	17	79971.4381	0.0086
17	9	8	17	17	←	17	9	9	17	17	79971.4381	0.0114

16	8	8	16	16	←	16	8	9	16	16	80011.0124	0.0423
16	9	8	16	16	←	16	7	9	16	16	80011.0124	0.0413
14	7	8	14	14	←	14	5	9	14	14	80071.8862	0.0092
14	6	8	14	14	←	14	6	9	14	14	80071.8862	0.0093
8	0	8	8	8	←	7	0	7	7	7	80114.9462	0.0159
8	1	8	8	8	←	7	1	7	7	7	80114.9462	0.0159
7	2	6	7	7	←	6	2	5	6	6	80120.4372	0.0162
7	1	6	7	7	←	6	1	5	6	6	80120.4372	0.0142
9	2	8	9	9	←	9	0	9	9	9	80149.0167	0.0279
9	1	8	9	9	←	9	1	9	9	9	80149.0167	0.0279
46	37	9	46	46	←	46	37	10	46	46	80950.3067	0.0492
45	36	9	45	45	←	45	36	10	45	45	82028.9189	-0.0002
44	35	9	44	44	←	44	35	10	44	44	82942.5027	-0.0182
45	37	9	45	45	←	45	35	10	45	45	83698.0733	0.0082
43	34	9	43	43	←	43	34	10	43	43	83721.5487	-0.0134
42	33	9	42	42	←	42	33	10	42	42	84391.2655	-0.0059
43	35	9	43	43	←	43	33	10	43	43	84516.2701	0.0241
41	32	9	41	41	←	41	32	10	41	41	84972.0188	0.0064
41	33	9	41	41	←	41	31	10	41	41	85330.4658	0.0279
40	31	9	40	40	←	40	31	10	40	40	85479.9325	-0.0045
40	32	9	40	40	←	40	30	10	40	40	85715.7372	0.006
39	30	9	39	39	←	39	30	10	39	39	85927.7334	0.0212
38	29	9	38	38	←	38	29	10	38	38	86325.2032	-0.0064
38	30	9	38	38	←	38	28	10	38	38	86422.9879	0.0095
37	29	9	37	37	←	37	27	10	37	37	86741.6627	-0.0199
36	28	9	36	36	←	36	26	10	36	36	87036.6143	0.0124
35	26	9	35	35	←	35	26	10	35	35	87284.8819	0.0006
35	27	9	35	35	←	35	25	10	35	35	87308.1815	0.0132
34	25	9	34	34	←	34	25	10	34	34	87543.2512	0.0105
34	26	9	34	34	←	34	24	10	34	34	87557.2155	0.0076
33	24	9	33	33	←	33	24	10	33	33	87776.5838	0.0229
33	25	9	33	33	←	33	23	10	33	33	87784.7863	-0.0043
32	23	9	32	32	←	32	23	10	32	32	87987.3249	-0.0371
31	22	9	31	31	←	31	22	10	31	31	88177.7727	0.0065
31	23	9	31	31	←	31	21	10	31	31	88180.4565	-0.0081
30	21	9	30	30	←	30	21	10	30	30	88349.5154	-0.08
30	22	9	30	30	←	30	20	10	30	30	88351.0871	-0.0066
29	20	9	29	29	←	29	20	10	29	29	88504.4349	-0.0093
29	21	9	29	29	←	29	19	10	29	29	88505.2573	-0.0004
26	18	9	26	26	←	26	16	10	26	26	88880.7031	-0.0276
25	16	9	25	25	←	25	16	10	25	25	88980.4961	0.0353
25	17	9	25	25	←	25	15	10	25	25	88980.4961	-0.0193
24	16	9	24	24	←	24	14	10	24	24	89069.2767	-0.0027
23	15	9	23	23	←	23	13	10	23	23	89147.9246	-0.0105
23	14	9	23	23	←	23	14	10	23	23	89147.9246	0.0012
22	14	9	22	22	←	22	12	10	22	22	89217.3331	-0.0072

22	13	9	22	22	←	22	13	10	22	22	89217.3331	-0.002
21	12	9	21	21	←	21	12	10	21	21	89278.3031	0.0035
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20	12	9	20	20	←	20	10	10	20	20	89331.5728	-0.0046
19	10	9	19	19	←	19	10	10	19	19	89377.892	0.0116
19	11	9	19	19	←	19	9	10	19	19	89377.892	0.0113
17	8	9	17	17	←	17	8	10	17	17	89452.2238	0.0145
17	9	9	17	17	←	17	7	10	17	17	89452.2238	0.0145
16	7	9	16	16	←	16	7	10	16	16	89481.465	0.0108
16	8	9	16	16	←	16	6	10	16	16	89481.465	0.0108
15	7	9	15	15	←	15	5	10	15	15	89506.1825	0.0129
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14	5	9	14	14	←	14	5	10	14	14	89526.8427	-0.0295
14	6	9	14	14	←	14	4	10	14	14	89526.8427	-0.0295
9	0	9	9	9	←	8	0	8	8	8	89539.6889	0.0157
9	1	9	9	9	←	8	1	8	8	8	89539.6889	0.0157
13	5	9	13	13	←	13	3	10	13	13	89544.0275	-0.0167
13	4	9	13	13	←	13	4	10	13	13	89544.0275	-0.0167
8	2	7	8	8	←	7	2	6	7	7	89544.9981	0.0162
8	1	7	8	8	←	7	1	6	7	7	89544.9981	0.0161
7	3	5	7	7	←	6	3	4	6	6	89552.7199	0.0247
12	4	9	12	12	←	12	2	10	12	12	89558.0743	-0.0591
12	3	9	12	12	←	12	3	10	12	12	89558.0743	-0.0591
11	3	9	11	11	←	11	1	10	11	11	89569.5167	-0.0376
11	2	9	11	11	←	11	2	10	11	11	89569.5167	-0.0376
49	39	10	49	49	←	49	39	11	49	49	91706.8735	0.0005
48	38	10	48	48	←	48	38	11	48	48	92451.374	-0.012
49	40	10	49	49	←	49	38	11	49	49	92568.7176	-0.0353
48	39	10	48	48	←	48	37	11	48	48	93042.3174	-0.002
47	38	10	47	47	←	47	36	11	47	47	93504.5952	-0.0252
46	36	10	46	46	←	46	36	11	46	46	93681.7033	-0.0068
46	37	10	46	46	←	46	35	11	46	46	93949.6701	0.0047
45	35	10	45	45	←	45	35	11	45	45	94196.3719	-0.0093
45	36	10	45	45	←	45	34	11	45	45	94373.546	0.002
44	34	10	44	44	←	44	34	11	44	44	94658.2725	0.0149
44	35	10	44	44	←	44	33	11	44	44	94773.9236	-0.0125
43	33	10	43	43	←	43	33	11	43	43	95075.1494	0.015
43	34	10	43	43	←	43	32	11	43	43	95149.6794	-0.0266
42	32	10	42	42	←	42	32	11	42	42	95453.119	-0.0129
42	33	10	42	42	←	42	31	11	42	42	95500.5379	-0.038
41	31	10	41	41	←	41	31	11	41	41	95797.08	-0.0101
41	32	10	41	41	←	41	30	11	41	41	95826.8715	0.0032
40	30	10	40	40	←	40	30	11	40	40	96110.8998	0.02
40	31	10	40	40	←	40	29	11	40	40	96129.3059	-0.0033

39	30	10	39	39	←	39	28	11	39	39	96408.8867	0.005
36	26	10	36	36	←	36	26	11	36	36	97119.6709	-0.0137
36	27	10	36	36	←	36	25	11	36	36	97122.0184	0.0114
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35	26	10	35	35	←	35	24	11	35	35	97321.9183	0.022
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34	25	10	34	34	←	34	23	11	34	34	97504.8638	0.0053
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33	23	10	33	33	←	33	23	11	33	33	97671.7922	0.1828
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29	20	10	29	29	←	29	18	11	29	29	98203.2073	-0.0211
29	19	10	29	29	←	29	19	11	29	29	98203.2073	0.0091
28	19	10	28	28	←	28	17	11	28	28	98306.3435	0.0095
28	18	10	28	28	←	28	18	11	28	28	98306.3435	0.0243
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27	17	10	27	27	←	27	17	11	27	27	98399.2752	0.0381
26	17	10	26	26	←	26	15	11	26	26	98482.6775	-0.0409
26	16	10	26	26	←	26	16	11	26	26	98482.6775	-0.0377
25	15	10	25	25	←	25	15	11	25	25	98557.4697	-0.0027
25	16	10	25	25	←	25	14	11	25	25	98557.4697	-0.0041
24	15	10	24	24	←	24	13	11	24	24	98624.1933	0.0053
24	14	10	24	24	←	24	14	11	24	24	98624.1933	0.006
23	13	10	23	23	←	23	13	11	23	23	98683.5572	0.0563
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22	13	10	22	22	←	22	11	11	22	22	98736.0346	0.0153
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21	12	10	21	21	←	21	10	11	21	21	98782.2984	-0.0164
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18	9	10	18	18	←	18	7	11	18	18	98889.1587	0.0238
17	8	10	17	17	←	17	6	11	17	17	98915.6547	-0.0094
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15	6	10	15	15	←	15	4	11	15	15	98957.7204	-0.0003
15	5	10	15	15	←	15	5	11	15	15	98957.7204	-0.0003
10	0	10	10	10	←	9	0	9	9	9	98964.363	0.0214
10	1	10	10	10	←	9	1	9	9	9	98964.363	0.0214
9	1	8	9	9	←	8	1	7	8	8	98969.5388	0.0027
9	2	8	9	9	←	8	2	7	8	8	98969.5388	0.0027
14	5	10	14	14	←	14	3	11	14	14	98974.0071	-0.0218

14	4	10	14	14	←	14	4	11	14	14	98974.0071	-0.0218
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13	3	10	13	13	←	13	3	11	13	13	98987.6454	-0.0236
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52	42	11	52	52	←	52	40	12	52	52	102073.7798	0.0203
51	40	11	51	51	←	51	40	12	51	51	102356.3109	-0.0347
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48	37	11	48	48	←	48	37	12	48	48	103789.607	0.0062
48	38	11	48	48	←	48	36	12	48	48	103845.543	0.0009
47	36	11	47	47	←	47	36	12	47	47	104188.8249	0.0226
47	37	11	47	47	←	47	35	12	47	47	104224.6644	-0.0203
46	35	11	46	46	←	46	35	12	46	46	104556.1631	0.0128
46	36	11	46	46	←	46	34	12	46	46	104578.921	0.0299
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44	33	11	44	44	←	44	33	12	44	44	105207.539	0.0079
44	34	11	44	44	←	44	32	12	44	44	105216.3368	0.0087
43	32	11	43	43	←	43	32	12	43	43	105496.3576	-0.068
43	33	11	43	43	←	43	31	12	43	43	105501.7875	-0.0031
42	31	11	42	42	←	42	31	12	42	42	105763.4251	-0.0001
42	32	11	42	42	←	42	30	12	42	42	105766.6514	-0.0011
41	30	11	41	41	←	41	30	12	41	41	106010.1977	0.0203
41	31	11	41	41	←	41	29	12	41	41	106012.0725	-0.0186
40	30	11	40	40	←	40	28	12	40	40	106239.2601	0.0059
39	29	11	39	39	←	39	27	12	39	39	106449.2544	0.0082
36	26	11	36	36	←	36	24	12	36	36	106986.416	-0.0533
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33	23	11	33	33	←	33	21	12	33	33	107403.915	-0.0094
31	20	11	31	31	←	31	20	12	31	31	107626.5066	-0.0068
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30	19	11	30	30	←	30	19	12	30	30	107723.2229	-0.0204
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28	18	11	28	28	←	28	16	12	28	28	107890.7471	-0.021
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17	7	11	17	17	←	17	5	12	17	17	108369.1359	0.0233
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11	0	11	11	11	←	10	0	10	10	10	108388.9572	0.0307
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26	3	24	26	26	←	25	2	23	25	25	268594.6404	-0.0004
25	4	22	25	25	←	24	4	21	24	24	268598.5732	0.0612
25	3	22	25	25	←	24	3	21	24	24	268598.5732	0.0612
25	4	22	25	25	←	24	3	21	24	24	268598.5732	0.0612
25	3	22	25	25	←	24	4	21	24	24	268598.5732	0.0612
24	5	20	24	24	←	23	4	19	23	23	268602.3571	-0.0186

24	5	20	24	24	←	23	5	19	23	23	268602.3571	-0.0186
24	4	20	24	24	←	23	5	19	23	23	268602.3571	-0.0186
24	4	20	24	24	←	23	4	19	23	23	268602.3571	-0.0186
23	5	18	23	23	←	22	6	17	22	22	268606.5196	-0.0714
23	6	18	23	23	←	22	5	17	22	22	268606.5196	-0.0714
23	6	18	23	23	←	22	6	17	22	22	268606.5196	-0.0714
23	5	18	23	23	←	22	5	17	22	22	268606.5196	-0.0714
21	8	14	21	21	←	20	7	13	20	20	268618.99	0.0094
21	7	14	21	21	←	20	7	13	20	20	268618.99	0.0094
21	7	14	21	21	←	20	8	13	20	20	268618.99	0.0094
21	8	14	21	21	←	20	8	13	20	20	268618.99	0.0094
20	9	12	20	20	←	19	9	11	19	19	268630.825	0.0296
20	9	12	20	20	←	19	8	11	19	19	268630.825	0.0296
20	8	12	20	20	←	19	9	11	19	19	268630.825	0.0296
20	8	12	20	20	←	19	8	11	19	19	268630.825	0.0296
19	10	10	19	19	←	18	9	9	18	18	268653.7923	0.0194
19	9	10	19	19	←	18	9	9	18	18	268653.7923	0.0194
19	9	10	19	19	←	18	10	9	18	18	268653.7923	0.0195
19	9	10	19	19	←	18	10	9	18	18	268653.7923	0.0195
18	11	8	18	18	←	17	11	7	17	17	268709.241	0.0371
18	10	8	18	18	←	17	11	7	17	17	268709.241	0.0444
29	1	29	29	29	←	28	1	28	28	28	278007.5927	0.0356
29	0	29	29	29	←	28	0	28	28	28	278007.5927	0.0356
29	1	29	29	29	←	28	0	28	28	28	278007.5944	0.0372
29	0	29	29	29	←	28	1	28	28	28	278007.5944	0.0372
28	1	27	28	28	←	27	1	26	27	27	278012.1271	0.0038
28	2	27	28	28	←	27	2	26	27	27	278012.1271	0.0038
28	1	27	28	28	←	27	2	26	27	27	278012.1284	0.005
28	2	27	28	28	←	27	1	26	27	27	278012.1284	0.005
27	2	25	27	27	←	26	3	24	26	26	278016.1862	-0.0191
27	3	25	27	27	←	26	2	24	26	26	278016.1862	-0.0191
27	2	25	27	27	←	26	2	24	26	26	278016.1863	-0.019
27	3	25	27	27	←	26	3	24	26	26	278016.1863	-0.019
26	3	23	26	26	←	25	3	22	25	25	278019.9735	-0.0201
26	4	23	26	26	←	25	4	22	25	25	278019.9735	-0.0201
26	4	23	26	26	←	25	3	22	25	25	278019.9736	-0.02
26	3	23	26	26	←	25	4	22	25	25	278019.9736	-0.02
25	5	21	25	25	←	24	5	20	24	24	278023.6981	-0.0254
25	4	21	25	25	←	24	4	20	24	24	278023.6981	-0.0254
25	4	21	25	25	←	24	5	20	24	24	278023.6999	-0.0236
25	5	21	25	25	←	24	4	20	24	24	278023.6999	-0.0236
24	6	19	24	24	←	23	6	18	23	23	278027.696	-0.023
24	5	19	24	24	←	23	5	18	23	23	278027.696	-0.023
24	5	19	24	24	←	23	6	18	23	23	278027.6985	-0.0205
24	6	19	24	24	←	23	5	18	23	23	278027.6985	-0.0205
23	6	17	23	23	←	22	6	16	22	22	278032.4996	0.0111

23	7	17	23	23	←	22	7	16	22	22	278032.4996	0.0111
23	6	17	23	23	←	22	7	16	22	22	278032.5012	0.0128
23	7	17	23	23	←	22	6	16	22	22	278032.5012	0.0128
22	7	15	22	22	←	21	7	14	21	21	278038.9299	-0.0169
22	8	15	22	22	←	21	8	14	21	21	278038.9299	-0.0169
22	8	15	22	22	←	21	7	14	21	21	278038.9316	-0.0153
22	7	15	22	22	←	21	8	14	21	21	278038.9316	-0.0153
21	8	13	21	21	←	20	8	12	20	20	278048.9519	-0.0427
21	9	13	21	21	←	20	9	12	20	20	278048.9519	-0.0427
21	8	13	21	21	←	20	9	12	20	20	278048.9547	-0.0399
21	9	13	21	21	←	20	8	12	20	20	278048.9547	-0.0399
44	14	30	44	44	←	44	14	31	44	44	287141.4504	-0.0095
44	15	30	44	44	←	44	13	31	44	44	287141.4504	-0.0095
41	12	30	41	41	←	41	10	31	41	41	287258.0626	0.0342
41	11	30	41	41	←	41	11	31	41	41	287258.0626	0.0342
30	0	30	30	30	←	29	1	29	29	29	287428.9723	0.0401
30	1	30	30	30	←	29	0	29	29	29	287428.9723	0.0401
30	1	30	30	30	←	29	1	29	29	29	287428.9723	0.0401
30	0	30	30	30	←	29	0	29	29	29	287428.9723	0.0401
29	1	28	29	29	←	28	2	27	28	28	287433.5167	0.0311
29	2	28	29	29	←	28	2	27	28	28	287433.5167	0.0311
29	2	28	29	29	←	28	1	27	28	28	287433.5167	0.0311
29	2	28	29	29	←	28	1	27	28	28	287433.5167	0.0311
29	1	28	29	29	←	28	1	27	28	28	287433.5167	0.0311
28	3	26	28	28	←	27	3	25	27	27	287437.5469	0.023
28	2	26	28	28	←	27	2	25	27	27	287437.5469	0.023
28	3	26	28	28	←	27	2	25	27	27	287437.5469	0.023
28	2	26	28	28	←	27	3	25	27	27	287437.5469	0.023
27	4	24	27	27	←	26	4	23	26	26	287441.2419	0.0089
27	3	24	27	27	←	26	3	23	26	26	287441.2419	0.0089
27	3	24	27	27	←	26	4	23	26	26	287441.2421	0.009
27	4	24	27	27	←	26	3	23	26	26	287441.2421	0.009
26	4	22	26	26	←	25	4	21	25	25	287444.8514	0.0151
26	5	22	26	26	←	25	5	21	25	25	287444.8514	0.0151
26	4	22	26	26	←	25	5	21	25	25	287444.8535	0.0172
26	5	22	26	26	←	25	4	21	25	25	287444.8535	0.0172
25	6	20	25	25	←	24	6	19	24	24	287448.6351	0.0045
25	5	20	25	25	←	24	5	19	24	24	287448.6351	0.0045
25	5	20	25	25	←	24	6	19	24	24	287448.6368	0.0063
25	6	20	25	25	←	24	5	19	24	24	287448.6368	0.0063
24	7	18	24	24	←	23	7	17	23	23	287453.0127	-0.047
24	6	18	24	24	←	23	6	17	23	23	287453.0127	-0.047
24	6	18	24	24	←	23	7	17	23	23	287453.0152	-0.0445
24	7	18	24	24	←	23	6	17	23	23	287453.0152	-0.0445
23	8	16	23	23	←	22	8	15	22	22	287458.9033	0.0213
23	7	16	23	23	←	22	7	15	22	22	287458.9033	0.0213

23	8	16	23	23	←	22	7	15	22	22	287458.905	0.023
23	7	16	23	23	←	22	8	15	22	22	287458.905	0.023
22	9	14	22	22	←	21	9	13	21	21	287467.5371	-0.0396
22	8	14	22	22	←	21	8	13	21	21	287467.5371	-0.0396
22	8	14	22	22	←	21	9	13	21	21	287467.5397	-0.037
22	9	14	22	22	←	21	8	13	21	21	287467.5397	-0.037
21	9	12	21	21	←	20	9	11	20	20	287482.4303	-0.0321
21	10	12	21	21	←	20	10	11	20	20	287482.4303	-0.0321
21	9	12	21	21	←	20	10	11	20	20	287482.433	-0.0294
21	10	12	21	21	←	20	9	11	20	20	287482.433	-0.0294
20	11	10	20	20	←	19	10	9	19	19	287512.2595	-0.005
20	11	10	20	20	←	19	11	9	19	19	287512.2595	-0.0047
20	10	10	20	20	←	19	10	9	19	19	287512.2595	-0.005
20	10	10	20	20	←	19	11	9	19	19	287512.2595	-0.0046
19	12	8	19	19	←	18	12	7	18	18	287585.2619	0.051

Table 8: Assigned transitions of the imidazole $^{13}\text{C}(5)$ isotopologue in the 2-8, 12-15.5, 18-26, 75-110 and 260-295 GHz regions. For transitions in the 75-110 and 260-295 GHz regions, the F quantum numbers become redundant due to the absence of hyperfine structure, and the F values are set to the values of the J quantum numbers.

J'	K'_a	K'_c	F'_1	F'_2		J	K_a	K_c	F_1	F_2	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
1	1	0	1	2	←	1	1	1	2	2	4512.3965	-0.0072
1	1	0	2	3	←	1	1	1	2	3	4513.2882	-0.003
2	1	1	3	3	←	2	1	2	3	3	13539.5452	-0.0094
2	1	1	3	4	←	2	1	2	3	4	13539.5452	-0.0251
1	0	1	0	1	←	0	0	0	1	2	13933.2328	0.0336
1	0	1	2	2	←	0	0	0	1	1	13933.5004	0.0176
1	0	1	1	0	←	0	0	0	1	1	13933.7897	0.0015
1	0	1	2	3	←	0	0	0	1	2	13934.5858	-0.0058
1	0	1	1	1	←	0	0	0	1	0	13934.5858	0.0807
1	0	1	1	2	←	0	0	0	1	1	13934.8808	-0.0163
1	1	1	2	1	←	0	0	0	1	2	14342.5472	0.0228
1	1	1	0	1	←	0	0	0	1	1	14343.1706	-0.0098
1	1	1	2	3	←	0	0	0	1	2	14343.389	-0.0049
1	1	1	2	2	←	0	0	0	1	1	14343.6054	-0.0078
1	1	1	1	2	←	0	0	0	1	2	14344.0389	-0.0502
1	1	1	1	1	←	0	0	0	1	0	14344.0389	0.0191
2	0	2	3	3	←	1	1	1	1	2	23327.9476	0.0243
2	0	2	3	3	←	1	1	1	2	2	23328.3887	-0.0105
2	0	2	3	4	←	1	1	1	2	3	23329.3624	0.0139
2	0	2	2	3	←	1	1	1	2	2	23329.9237	0.0254
2	1	2	1	2	←	1	1	1	1	2	23354.5668	0.0216
2	1	2	3	3	←	1	1	1	1	2	23354.5668	0.0175
2	1	2	1	2	←	1	1	1	2	2	23355.0089	-0.0122
2	1	2	3	2	←	1	1	1	1	1	23355.4044	0.1051
2	1	2	1	2	←	1	1	1	0	1	23355.4044	-0.0494
2	1	2	2	2	←	1	1	1	1	2	23355.9148	0.0249
2	1	2	2	3	←	1	1	1	2	2	23356.4818	0.0281
2	1	2	2	3	←	1	1	1	2	2	23356.4818	0.0281
2	1	2	3	2	←	1	1	1	2	1	23356.8434	0.0486
2	1	2	2	2	←	1	1	1	0	1	23356.8434	0.0448
3	1	2	3	4	←	3	1	3	3	4	23471.2342	-0.0128
3	1	2	3	4	←	3	1	3	4	5	23472.2587	-0.0149
3	1	2	3	3	←	3	1	3	4	4	23472.9771	0.0047
2	0	2	1	2	←	1	0	1	1	2	23737.09	-0.0581
2	0	2	2	2	←	1	0	1	2	1	23737.09	0.1144
2	0	2	3	3	←	1	0	1	2	3	23737.4279	0.0071
2	0	2	1	1	←	1	0	1	0	1	23738.6101	0.1291
2	0	2	3	3	←	1	0	1	2	2	23738.6101	0.0805
2	0	2	2	3	←	1	0	1	1	2	23738.6101	-0.0042

2	0	2	1	2	←	1	0	1	0	1	23738.6101	-0.236
2	0	2	3	2	←	1	0	1	0	1	23739.5272	-0.0247
2	0	2	1	0	←	1	0	1	0	1	23739.5272	0.0055
2	0	2	2	2	←	1	0	1	2	2	23739.9495	-0.0159
2	1	2	3	4	←	1	0	1	2	3	23764.7129	0.0114
37	30	8	37	37	←	37	28	9	37	37	74885.8628	-0.0366
35	28	8	35	35	←	35	26	9	35	35	74902.203	0.0255
34	27	8	34	34	←	34	25	9	34	34	75162.6094	-0.0118
33	26	8	33	33	←	33	24	9	33	33	75513.5859	-0.0496
31	23	8	31	31	←	31	23	9	31	31	75634.2471	0.0108
32	25	8	32	32	←	32	23	9	32	32	75913.8564	0.0033
30	22	8	30	30	←	30	22	9	30	30	76322.9469	0.0155
31	24	8	31	31	←	31	22	9	31	31	76332.9828	-0.0002
30	23	8	30	30	←	30	21	9	30	30	76749.7607	-0.003
29	21	8	29	29	←	29	21	9	29	29	76895.2624	0.0151
29	22	8	29	29	←	29	20	9	29	29	77150.0307	-0.0171
28	20	8	28	28	←	28	20	9	28	28	77376.5772	0.0007
28	21	8	28	28	←	28	19	9	28	28	77525.0814	-0.0191
27	19	8	27	27	←	27	19	9	27	27	77785.7055	-0.0023
27	20	8	27	27	←	27	18	9	27	27	77870.1492	-0.0054
26	18	8	26	26	←	26	18	9	26	26	78136.4156	-0.0477
26	19	8	26	26	←	26	17	9	26	26	78183.233	-0.0015
38	32	7	38	38	←	38	30	8	38	38	78382.5847	0.0248
25	17	8	25	25	←	25	17	9	25	25	78439.0353	-0.0112
25	18	8	25	25	←	25	16	9	25	25	78464.2236	-0.016
24	16	8	24	24	←	24	16	9	24	24	78701.1033	0.017
24	17	8	24	24	←	24	15	9	24	24	78714.2516	-0.0067
23	16	8	23	23	←	23	14	9	23	23	78935.1225	0.0467
22	15	8	22	22	←	22	13	9	22	22	79128.7971	-0.0399
21	13	8	21	21	←	21	13	9	21	21	79296.2923	0.0028
21	14	8	21	21	←	21	12	9	21	21	79297.8031	-0.0222
18	11	8	18	18	←	18	9	9	18	18	79678.5357	-0.0405
18	10	8	18	18	←	18	10	9	18	18	79678.5357	0.0819
16	8	8	16	16	←	16	8	9	16	16	79847.7787	0.0518
16	9	8	16	16	←	16	7	9	16	16	79847.7787	0.0348
15	8	8	15	15	←	15	6	9	15	15	79912.3952	0.0196
15	7	8	15	15	←	15	7	9	15	15	79912.3952	0.0253
13	5	8	13	13	←	13	5	9	13	13	80009.4513	-0.0394
13	6	8	13	13	←	13	4	9	13	13	80009.4513	-0.0399
8	0	8	8	8	←	7	0	7	7	7	80083.1272	0.0097
8	1	8	8	8	←	7	1	7	7	7	80083.1272	0.0097
7	2	6	7	7	←	6	2	5	6	6	80089.0567	-0.0082
7	1	6	7	7	←	6	1	5	6	6	80089.0567	-0.02
38	29	9	38	38	←	38	29	10	38	38	81681.5745	0.013
41	33	9	41	41	←	41	31	10	41	41	82579.8752	-0.0219
40	32	9	40	40	←	40	30	10	40	40	82780.4674	-0.0216

37	28	9	37	37	←	37	28	10	37	37	82817.1895	0.0126
39	31	9	39	39	←	39	29	10	39	39	83122.827	-0.0145
38	30	9	38	38	←	38	28	10	38	38	83553.3243	-0.0015
36	27	9	36	36	←	36	27	10	36	36	83754.359	0.0022
36	28	9	36	36	←	36	26	10	36	36	84526.6613	-0.0074
35	26	9	35	35	←	35	26	10	35	35	84536.7603	0.0113
35	27	9	35	35	←	35	25	10	35	35	85018.6286	0.0378
34	25	9	34	34	←	34	25	10	34	34	85198.1275	0.023
34	26	9	34	34	←	34	24	10	34	34	85492.8928	0.0335
33	24	9	33	33	←	33	24	10	33	33	85763.9051	-0.0018
33	25	9	33	33	←	33	23	10	33	33	85940.6229	0.0036
32	24	9	32	32	←	32	22	10	32	32	86356.9113	0.0128
31	23	9	31	31	←	31	21	10	31	31	86739.4841	0.0081
30	21	9	30	30	←	30	21	10	30	30	87054.4877	-0.0114
29	21	9	29	29	←	29	19	10	29	29	87403.2623	-0.0623
28	20	9	28	28	←	28	18	10	28	28	87687.0095	-0.023
27	18	9	27	27	←	27	18	10	27	27	87935.9361	-0.0414
26	17	9	26	26	←	26	17	10	26	26	88165.085	0.0001
26	18	9	26	26	←	26	16	10	26	26	88167.6537	-0.0247
25	16	9	25	25	←	25	16	10	25	25	88367.678	0.0013
25	17	9	25	25	←	25	15	10	25	25	88368.896	-0.0539
24	15	9	24	24	←	24	15	10	24	24	88546.4519	0.0095
22	13	9	22	22	←	22	13	10	22	22	88841.6709	0.0518
22	14	9	22	22	←	22	12	10	22	22	88841.6709	-0.0701
21	12	9	21	21	←	21	12	10	21	21	88962.0225	0.0271
21	13	9	21	21	←	21	11	10	21	21	88962.0225	-0.0243
20	12	9	20	20	←	20	10	10	20	20	89066.5826	-0.0084
20	11	9	20	20	←	20	11	10	20	20	89066.5826	0.0122
19	11	9	19	19	←	19	9	10	19	19	89156.9423	0.018
19	10	9	19	19	←	19	10	10	19	19	89156.9423	0.0258
18	9	9	18	18	←	18	9	10	18	18	89234.5018	0.0171
18	10	9	18	18	←	18	8	10	18	18	89234.5018	0.0143
17	8	9	17	17	←	17	8	10	17	17	89300.6499	0.032
17	9	9	17	17	←	17	7	10	17	17	89300.6499	0.0311
16	8	9	16	16	←	16	6	10	16	16	89356.5786	0.0168
16	7	9	16	16	←	16	7	10	16	16	89356.5786	0.0171
15	7	9	15	15	←	15	5	10	15	15	89403.4564	-0.0142
15	6	9	15	15	←	15	6	10	15	15	89403.4564	-0.0142
14	5	9	14	14	←	14	5	10	14	14	89442.3842	-0.0329
14	6	9	14	14	←	14	4	10	14	14	89442.3842	-0.0329
13	4	9	13	13	←	13	4	10	13	13	89474.3324	-0.0617
13	5	9	13	13	←	13	3	10	13	13	89474.3324	-0.0617
9	0	9	9	9	←	8	0	8	8	8	89504.1239	0.0158
9	1	9	9	9	←	8	1	8	8	8	89504.1239	0.0158
8	2	7	8	8	←	7	2	6	7	7	89509.6851	-0.0309
8	1	7	8	8	←	7	1	6	7	7	89509.6851	-0.0314

44	35	10	44	44	←	44	33	11	44	44	90979.76	-0.0065
43	34	10	43	43	←	43	32	11	43	43	91488.3655	0.0256
43	34	10	43	43	←	43	32	11	43	43	91488.3655	0.0256
41	31	10	41	41	←	41	31	11	41	41	91780.855	-0.0272
42	33	10	42	42	←	42	31	11	42	42	92041.8695	-0.0327
41	32	10	41	41	←	41	30	11	41	41	92611.1841	0.0132
40	30	10	40	40	←	40	30	11	40	40	92648.9596	0.0381
40	31	10	40	40	←	40	29	11	40	40	93175.4491	0.0044
39	29	10	39	39	←	39	29	11	39	39	93392.5858	-0.0111
39	30	10	39	39	←	39	28	11	39	39	93720.7773	0.0151
38	28	10	38	38	←	38	28	11	38	38	94037.3334	0.0175
38	29	10	38	38	←	38	27	11	38	38	94238.3143	0.0196
37	27	10	37	37	←	37	27	11	37	37	94602.1085	0.0112
37	28	10	37	37	←	37	26	11	37	37	94723.004	0.0072
36	26	10	36	36	←	36	26	11	36	36	95101.1173	-0.0008
36	27	10	36	36	←	36	25	11	36	36	95172.516	-0.0016
35	25	10	35	35	←	35	25	11	35	35	95544.9651	-0.0157
35	26	10	35	35	←	35	24	11	35	35	95586.3645	0.0134
34	24	10	34	34	←	34	24	11	34	34	95941.6987	0.0029
34	25	10	34	34	←	34	23	11	34	34	95965.2073	0.0113
33	23	10	33	33	←	33	23	11	33	33	96297.4206	0.0044
33	24	10	33	33	←	33	22	11	33	33	96310.4892	-0.0028
32	22	10	32	32	←	32	22	11	32	32	96616.983	0.0087
32	23	10	32	32	←	32	21	11	32	32	96624.1077	0.0142
31	22	10	31	31	←	31	20	11	31	31	96908.1068	0.0565
30	20	10	30	30	←	30	20	11	30	30	97162.5133	0.0152
30	21	10	30	30	←	30	19	11	30	30	97164.4427	-0.023
29	19	10	29	29	←	29	19	11	29	29	97394.4128	-0.0013
29	20	10	29	29	←	29	18	11	29	29	97395.401	-0.0091
28	19	10	28	28	←	28	17	11	28	28	97602.6559	-0.2155
28	18	10	28	28	←	28	18	11	28	28	97602.6559	0.2749
26	16	10	26	26	←	26	16	11	26	26	97954.6879	0.0428
24	15	10	24	24	←	24	13	11	24	24	98233.7705	-0.0027
24	14	10	24	24	←	24	14	11	24	24	98233.7705	0.0181
23	13	10	23	23	←	23	13	11	23	23	98349.7194	-0.0122
23	14	10	23	23	←	23	12	11	23	23	98349.7194	-0.0209
22	12	10	22	22	←	22	12	11	22	22	98451.7973	-0.0254
22	13	10	22	22	←	22	11	11	22	22	98451.7973	-0.0288
21	11	10	21	21	←	21	11	11	21	21	98541.2843	0.0079
21	12	10	21	21	←	21	10	11	21	21	98541.2843	0.0066
20	11	10	20	20	←	20	9	11	20	20	98619.2397	-0.0199
20	10	10	20	20	←	20	10	11	20	20	98619.2397	-0.0194
19	10	10	19	19	←	19	8	11	19	19	98686.8457	-0.0158
19	9	10	19	19	←	19	9	11	19	19	98686.8457	-0.0156
17	7	10	17	17	←	17	7	11	17	17	98794.9877	0.0546
17	8	10	17	17	←	17	6	11	17	17	98794.9877	0.0546

16	7	10	16	16	←	16	5	11	16	16	98837.2478	0.0014
16	6	10	16	16	←	16	6	11	16	16	98837.2478	0.0014
15	5	10	15	15	←	15	5	11	15	15	98872.8395	-0.034
15	6	10	15	15	←	15	4	11	15	15	98872.8395	-0.034
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10	0	10	10	10	←	9	0	9	9	9	98925.0406	0.0143
13	3	10	13	13	←	13	3	11	13	13	98927.0707	-0.0482
9	1	8	9	9	←	8	1	7	8	8	98930.4312	0.003
9	2	8	9	9	←	8	2	7	8	8	98930.4312	0.003
8	3	6	8	8	←	7	3	5	7	7	98938.8528	0.0773
8	2	6	8	8	←	7	2	5	7	7	98938.8528	0.0069
12	3	10	12	12	←	12	1	11	12	12	98947.1123	-0.0163
42	31	11	42	42	←	42	31	12	42	42	102846.0885	0.0154
42	32	11	42	42	←	42	30	12	42	42	102981.7584	-0.0074
41	30	11	41	41	←	41	30	12	41	41	103413.7737	-0.0171
41	31	11	41	41	←	41	29	12	41	41	103495.642	0.0021
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39	28	11	39	39	←	39	28	12	39	39	104384.3888	0.0174
39	29	11	39	39	←	39	27	12	39	39	104412.7154	0.0214
38	27	11	38	38	←	38	27	12	38	38	104801.5945	0.0051
37	27	11	37	37	←	37	25	12	37	37	105189.5482	-0.0108
35	24	11	35	35	←	35	24	12	35	35	105838.144	0.0183
35	25	11	35	35	←	35	23	12	35	35	105840.8239	-0.0284
34	23	11	34	34	←	34	23	12	34	34	106123.061	0.0338
34	24	11	34	34	←	34	22	12	34	34	106124.4404	-0.0312
33	22	11	33	33	←	33	22	12	33	33	106381.9389	-0.0101
33	23	11	33	33	←	33	21	12	33	33	106382.6919	-0.0055
32	21	11	32	32	←	32	21	12	32	32	106617.0084	0.0055
32	22	11	32	32	←	32	20	12	32	32	106617.409	0.0273
30	19	11	30	30	←	30	19	12	30	30	107022.9413	0.0484
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29	18	11	29	29	←	29	18	12	29	29	107197.0438	0.0327
29	19	11	29	29	←	29	17	12	29	29	107197.0438	-0.0092
28	17	11	28	28	←	28	17	12	28	28	107353.8905	0.0108
28	18	11	28	28	←	28	16	12	28	28	107353.8905	-0.0081
26	16	11	26	26	←	26	14	12	26	26	107621.1282	-0.0102
26	15	11	26	26	←	26	15	12	26	26	107621.1282	-0.0067
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22	12	11	22	22	←	22	10	12	22	22	108001.8968	-0.0205
22	11	11	22	22	←	22	11	12	22	22	108001.8968	-0.0204
21	11	11	21	21	←	21	9	12	21	21	108070.9579	-0.0242
21	10	11	21	21	←	21	10	12	21	21	108070.9579	-0.0242

20	10	11	20	20	←	20	8	12	20	20	108131.3552	-0.0224
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19	9	11	19	19	←	19	7	12	19	19	108183.8613	-0.0422
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15	4	11	15	15	←	15	4	12	15	15	108329.6999	0.0059
15	5	11	15	15	←	15	3	12	15	15	108329.6999	0.0059
11	0	11	11	11	←	10	0	10	10	10	108345.8559	-0.0061
11	1	11	11	11	←	10	1	10	10	10	108345.8559	-0.0061
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36	8	28	36	36	←	36	8	29	36	36	268365.853	0.1005
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28	0	28	28	28	←	27	0	27	27	27	268479.0904	-0.0233
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27	1	26	27	27	←	26	2	25	26	26	268483.6975	0.0126
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26	3	24	26	26	←	25	2	23	25	25	268487.8216	-0.0302
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22	7	16	22	22	←	21	6	15	21	21	268508.0676	-0.0177
22	6	16	22	22	←	21	6	15	21	21	268508.0692	-0.0161

22	7	16	22	22	←	21	7	15	21	21	268508.0692	-0.0161
21	8	14	21	21	←	20	7	13	20	20	268518.9313	-0.0963
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19	10	10	19	19	←	18	10	9	18	18	268581.2168	0.0262
19	9	10	19	19	←	18	9	9	18	18	268581.218	0.0248
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17	12	6	17	17	←	16	12	5	16	16	268924.9432	0.0661
29	0	29	29	29	←	28	1	28	28	28	277896.9893	0.0037
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28	1	27	28	28	←	27	2	26	27	27	277901.4963	-0.0429
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27	2	25	27	27	←	26	3	24	26	26	277905.6106	-0.0436
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26	3	23	26	26	←	25	4	22	25	25	277909.555	-0.0209
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26	4	23	26	26	←	25	4	22	25	25	277909.5566	-0.0193
26	3	23	26	26	←	25	3	22	25	25	277909.5566	-0.0193
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23	7	17	23	23	←	22	7	16	22	22	277924.6281	-0.0179
21	9	13	21	21	←	20	8	12	20	20	277950.6728	-0.0599
21	8	13	21	21	←	20	9	12	20	20	277950.6728	-0.0599
21	8	13	21	21	←	20	8	12	20	20	277950.6756	-0.057
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19	10	9	19	19	←	18	11	8	18	18	278059.5954	0.0618

19	11	9	19	19	←	18	10	8	18	18	278059.5954	-0.0654
19	11	9	19	19	←	18	11	8	18	18	278059.5961	0.0548
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30	0	30	30	30	←	29	1	29	29	29	287314.6381	0.0325
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28	3	26	28	28	←	27	2	25	27	27	287323.2748	0.0641
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28	3	26	28	28	←	27	3	25	27	27	287323.2763	0.0656
27	4	24	27	27	←	26	3	23	26	26	287327.0124	-0.0263
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26	5	22	26	26	←	25	4	21	25	25	287330.9524	0.0112
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26	4	22	26	26	←	25	4	21	25	25	287330.954	0.0127
25	5	20	25	25	←	24	6	19	24	24	287335.3564	-0.0231
25	6	20	25	25	←	24	5	19	24	24	287335.3564	-0.0231
25	5	20	25	25	←	24	5	19	24	24	287335.3581	-0.0214
25	6	20	25	25	←	24	6	19	24	24	287335.3581	-0.0214
24	6	18	24	24	←	23	7	17	23	23	287341.1271	0.0125
24	7	18	24	24	←	23	6	17	23	23	287341.1271	0.0125
24	6	18	24	24	←	23	6	17	23	23	287341.1282	0.0136
24	7	18	24	24	←	23	7	17	23	23	287341.1282	0.0136
23	7	16	23	23	←	22	8	15	22	22	287349.5892	0.0449
23	8	16	23	23	←	22	7	15	22	22	287349.5892	0.0449
23	7	16	23	23	←	22	7	15	22	22	287349.5895	0.0453
23	8	16	23	23	←	22	8	15	22	22	287349.5895	0.0453
22	9	14	22	22	←	21	8	13	21	21	287363.5189	-0.0148
22	8	14	22	22	←	21	9	13	21	21	287363.5189	-0.0148
22	8	14	22	22	←	21	8	13	21	21	287363.5214	-0.0123
22	9	14	22	22	←	21	9	13	21	21	287363.5214	-0.0123
21	9	12	21	21	←	20	10	11	20	20	287389.7391	0.0354
21	10	12	21	21	←	20	9	11	20	20	287389.7391	0.0353
21	10	12	21	21	←	20	10	11	20	20	287389.7394	0.0356
21	9	12	21	21	←	20	9	11	20	20	287389.7394	0.0356
18	12	6	18	18	←	17	12	5	17	17	288394.5555	-0.0103

B. The Anharmonic Energies of the First Ten Fundamental Vibrational Modes of Imidazole

Table 9: The anharmonic energies of the lowest ten normal modes of imidazole obtained using the hybrid approach detailed in Section 2 of the main manuscript.

Mode	$\Delta E^a / \text{cm}^{-1}$
ν_{21}	498.6
ν_{20}	628.0
ν_{19}	663.2
ν_{18}	724.2
ν_{17}	810.2
ν_{16}	857.2
ν_{15}	887.9
ν_{14}	919.9
ν_{13}	1054.3
ν_{12}	1073.9

C. Coordinates of Heavy Atoms in Imidazole from the r_s Structure Analysis

Table 10: The coordinates of the heavy atoms in imidazole obtained from the r_s structure.

atom	x	y	z
¹⁵ N(1)	-1.00895	-0.50549	0.0000
¹³ C(2)	0.22444	-1.08961	0.0000
¹⁵ N(3)	1.18992	-0.18816	0.0000
¹³ C(4)	0.54671	1.02471	0.0000
¹³ C(5)	-0.81275	0.85531	0.0000

D. Comparison of τ'_{aaaa} and τ'_{bbbb} Values for the Imiadzole Isotopologues

Table 11: A comparison between the τ'_{aaaa} and τ'_{bbbb} values from this work and those determined by Christen *et al.* [2].

Isotopologue	τ'_{aaaa}		τ'_{bbbb}	
	This work	Christen <i>et al.</i> [2]	This work	Christen <i>et al.</i> [2]
$^{15}\text{N}(1)$	-13.23030(201)	-13.73(61)	-12.16344(201)	-13.63(51)
$^{13}\text{C}(2)$	-12.50712(269)	-11.96(14)	-12.50712(269)	-13.77(13)
$^{15}\text{N}(3)$	-13.14752(807)	-14.20(75)	-13.14752(807)	-14.53(75)
$^{13}\text{C}(4)$	-13.20630(142)	-14.68(62)	-13.20630(142)	-13.96(70)
$^{13}\text{C}(5)$	-12.83072(185)	-12.74(79)	-12.83072(185)	-13.63(62)

E. Comparison of Errors in the Structural Parameters of Imidazole

Table 12: A comparison between the bond lengths, including error analysis, determined in this work and in Christen *et al.* [2]. Both sets of parameters were determined using the KRA method. The values tabulated in the Christen *et al.* column were re-determined by inputting the reported rotational constants and associated errors into the KRA programme [3].

Bond length / Å	This work	Christen <i>et al.</i> (1982) [2]
N(1)-C(2)	1.36472 ± 0.00634	1.36434 ± 0.00636
C(2)-N(3)	1.32090 ± 0.00743	1.32091 ± 0.00745
N(3)-C(4)	1.37287 ± 0.00730	1.37258 ± 0.00733
C(4)-C(5)	1.36997 ± 0.00329	1.36380 ± 0.00331
N(1)-C(5)	1.37487 ± 0.00343	1.37743 ± 0.00346

Table 13: A comparison between the internal bond angles of the imidazole ring, including error analysis, determined in this work and in Christen *et al.* [2]. Both sets of parameters were determined using the KRA method. The values tabulated in the Christen *et al.* column were re-determined by inputting the reported rotational constants and associated errors into the KRA programme [3].

Bond angle / °	This work	Christen <i>et al.</i> (1982) [2]
N(1)-C(2)-N(3)	111.62258 ± 0.30643	111.64454 ± 0.30781
C(2)-N(3)-C(4)	105.09777 ± 0.26160	105.06975 ± 0.26236
N(3)-C(4)-C(5)	110.83501 ± 0.21756	110.90306 ± 0.21936
C(4)-C(5)-N(1)	105.30728 ± 0.14910	105.48089 ± 0.15137
C(5)-N(1)-C(2)	107.13736 ± 0.19968	106.90176 ± 0.20028

F. Experimentally Determined Rotational Constants for the Isotopologues of Hydantoin

Table 14: Experimentally determined rotational constants for the isotopologues of hydantoin. Values in square brackets were kept fixed to the parent values reported in Ref. [4].

	$^{15}\text{N}(1)$	$^{13}\text{C}(2)$	$^{15}\text{N}(3)$	$^{13}\text{C}(4)$	$^{13}\text{C}(5)$
<i>A</i>	/ MHz	6466.5481(21)	6536.0124(20)	6429.0550(20)	6402.2796(19)
<i>B</i>	/ MHz	2291.4408(22)	2277.9082(16)	2285.7355(17)	2286.2670(25)
<i>C</i>	/ MHz	1711.57234(93)	1708.77738(80)	1705.7606(11)	1704.13883(86)
$\chi_{cc}^{(1)}$	/ MHz	-	1.53(9)	1.634(41)	1.56(8)
$\chi_{bb}^{(1)} - \chi_{aa}^{(1)}$	/ MHz	-	5.048(144)	5.324(48)	5.260(184)
$\chi_{cc}^{(3)}$	/ MHz	2.600(43)	2.606(63)	-	2.484(53)
$\chi_{bb}^{(3)} - \chi_{aa}^{(3)}$	/ MHz	6.816(56)	7.096(116)	-	6.936(152)
No. of lines		21	25	21	28
σ	/ kHz	26.7	20.2	23.3	24.1
					24.0

G. Assigned Transitions for the Isotopologues of Hydantoin

Tables detailing the assigned transitions for each of the reported isotopologues of hydantoin. The tables contain quantum numbers, experimental frequencies, and the observed minus calculated frequencies, and the tables are the product of the fitting procedure with the SPFIT programme [1].

Table 15: Assigned transitions of the hydantoin $^{15}\text{N}(1)$ isotopologue in the 18-26 GHz region.

J'	K'_a	K'_c	F'		J	K_a	K_c	F	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
8	3	5	7	←	8	2	6	7	18062.7569	0.0250
8	3	5	9	←	8	2	6	9	18062.7569	-0.0119
5	1	5	4	←	4	0	4	3	20592.9847	0.0606
5	1	5	6	←	4	0	4	5	20592.9847	0.0031
5	1	5	5	←	4	0	4	4	20593.6384	-0.0164
6	0	6	6	←	5	1	5	5	20877.9467	-0.0155
6	0	6	5	←	5	1	5	4	20878.1924	-0.0020
2	2	1	1	←	1	1	0	0	21109.5326	0.0202
2	2	1	2	←	1	1	0	2	21110.3248	-0.0064
2	2	1	3	←	1	1	0	2	21111.1715	0.0045
2	2	1	2	←	1	1	0	1	21111.7589	0.0150
4	3	1	4	←	4	2	2	4	21717.9346	0.0375
4	3	1	3	←	4	2	2	3	21718.1803	0.0003
2	2	0	2	←	1	1	1	1	21746.0888	-0.0160
2	2	0	3	←	1	1	1	2	21747.7209	0.0117
2	2	0	1	←	1	1	1	0	21749.1993	0.0011
3	3	1	3	←	3	2	2	4	22357.9566	-0.0378
3	3	1	4	←	3	2	2	3	22359.0523	-0.0667
3	3	1	2	←	3	2	2	2	22359.5101	-0.0027
6	1	6	5	←	5	0	5	4	23487.1790	-0.0158
6	1	6	7	←	5	0	5	6	23487.1790	-0.0414
6	1	6	6	←	5	0	5	5	23487.7230	-0.0103
3	2	2	3	←	2	1	1	3	24534.2740	0.0631
3	2	2	3	←	2	1	1	2	24534.9071	0.0185

Table 16: Assigned transitions of the hydantoin $^{13}\text{C}(2)$ isotopologue in the 18-26 GHz region.

J'	K'_a	K'_c	F'_1	F'_2		J	K_a	K_c	F_1	F_2	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
5	1	5	6	7	←	4	0	4	5	6	20645.5040	0.0131
5	1	5	4	5	←	4	0	4	3	4	20645.5040	0.0685
5	1	5	6	5	←	4	0	4	5	4	20645.5040	0.0779
5	1	5	4	3	←	4	0	4	3	2	20645.5040	0.1328
5	1	5	6	6	←	4	0	4	5	5	20646.1821	-0.0412
5	1	5	4	4	←	4	0	4	3	3	20646.1821	0.0192
5	1	5	5	5	←	4	0	4	4	4	20646.7346	0.0099
6	0	6	7	8	←	5	1	5	6	7	20755.5062	-0.0904
6	0	6	6	7	←	5	1	5	5	6	20755.5062	-0.0020
7	1	6	7	6	←	6	2	5	6	5	20816.3961	0.0155
2	2	1	3	2	←	1	1	0	2	1	21314.8035	0.0093
2	2	1	1	2	←	1	1	0	0	1	21316.3363	0.0086
2	2	1	3	4	←	1	1	0	2	3	21316.7706	0.0671
2	2	1	2	3	←	1	1	0	2	2	21316.7706	-0.1201
2	2	1	2	2	←	1	1	0	1	1	21317.1949	0.0192
2	2	1	3	3	←	1	1	0	1	2	21317.5982	-0.0294
2	2	0	3	3	←	1	1	1	1	2	21937.8061	-0.0019
2	2	0	2	3	←	1	1	1	2	2	21939.0465	-0.0097
2	2	0	3	4	←	1	1	1	2	3	21939.8070	-0.0082
2	2	0	1	2	←	1	1	1	2	2	21939.8070	0.0668
2	2	0	1	2	←	1	1	1	2	1	21940.3447	0.0217
3	3	0	4	4	←	3	2	1	4	4	22484.2795	-0.0064
3	3	0	4	3	←	3	2	1	4	3	22485.3751	-0.0005
6	1	6	7	8	←	5	0	5	6	7	23526.7792	-0.0472
6	1	6	5	6	←	5	0	5	4	5	23526.7792	-0.0166
6	1	6	7	6	←	5	0	5	6	5	23526.7792	-0.0120
6	1	6	5	4	←	5	0	5	4	3	23526.7792	0.0145
6	1	6	6	7	←	5	0	5	5	6	23527.2017	-0.0162
6	1	6	6	5	←	5	0	5	5	4	23527.2017	0.0154
6	1	6	7	7	←	5	0	5	6	6	23527.3691	-0.0091
6	1	6	5	5	←	5	0	5	4	4	23527.3691	0.0248
6	1	6	6	6	←	5	0	5	5	5	23527.7787	0.0035
3	2	2	2	2	←	2	1	1	1	1	24733.8507	-0.0072
3	2	2	3	2	←	2	1	1	1	2	24733.8507	-0.0291
3	2	2	4	5	←	2	1	1	3	4	24734.0731	-0.0107
3	2	2	3	4	←	2	1	1	3	3	24734.5000	0.0000
3	2	2	4	4	←	2	1	1	2	3	24734.9778	0.0243
3	2	2	3	3	←	2	1	1	2	2	24735.2406	-0.0019

Table 17: Assigned transitions of the hydantoin $^{15}\text{N}(3)$ isotopologue in the 18-26 GHz region.

J'	K'_a	K'_c	F'		J	K_a	K_c	F	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
6	1	6	6	←	4	0	4	3	20506.2388	0.0716
6	1	6	7	←	4	0	4	5	20506.2388	0.0183
6	1	6	5	←	4	0	4	4	20506.7678	0.0143
5	1	5	5	←	1	1	0	0	20991.5729	-0.0215
5	1	5	4	←	1	1	0	2	20992.3859	0.0425
5	1	5	6	←	1	1	0	2	20992.8607	-0.0079
2	2	1	3	←	1	1	0	1	20993.3718	-0.0154
2	2	1	2	←	1	1	0	1	20994.2523	0.0478
2	2	1	1	←	4	2	2	3	21555.4066	-0.0259
2	2	1	2	←	4	2	2	5	21555.4066	-0.0079
2	2	1	1	←	1	1	1	1	21628.6584	-0.0123
2	2	0	3	←	1	1	1	2	21629.2384	0.0140
2	2	0	1	←	1	1	1	2	21629.8443	-0.0131
2	2	0	2	←	1	1	1	0	21631.0036	-0.0363
2	2	0	2	←	7	1	7	7	21834.5001	-0.0197
3	2	2	3	←	6	2	5	6	23112.3364	0.0243
3	2	2	4	←	5	0	5	6	23392.2851	-0.0219
3	2	2	2	←	5	0	5	4	23392.2851	0.0028
8	2	7	8	←	5	0	5	5	23392.6848	-0.0255
8	2	7	9	←	8	1	8	8	24257.6186	0.0200
6	3	4	6	←	8	1	8	9	24258.6614	-0.0049
7	2	6	7	←	2	1	1	1	24403.9652	-0.0204
4	3	1	3	←	2	1	1	3	24404.3247	0.0093
4	3	1	5	←	2	1	1	2	24404.9060	-0.0026

Table 18: Assigned transitions of the hydantoin $^{13}\text{C}(4)$ isotopologue in the 18-26 GHz region.

J'	K'_a	K'_c	F'_1	F'_2		J	K_a	K_c	F_1	F_2	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
5	1	5	4	5	←	4	0	4	3	4	20464.1791	0.0242
5	1	5	6	5	←	4	0	4	5	4	20464.1791	0.0289
5	1	5	6	7	←	4	0	4	5	6	20464.1791	-0.0307
5	1	5	4	3	←	4	0	4	3	2	20464.1791	0.0825
5	1	5	6	6	←	4	0	4	5	5	20464.7924	-0.1187
5	1	5	5	6	←	4	0	4	4	5	20464.7924	0.0764
5	1	5	4	4	←	4	0	4	3	3	20464.7924	-0.0587
5	1	5	4	4	←	4	0	4	5	5	20464.7924	0.1150
5	1	5	5	5	←	4	0	4	4	4	20465.4523	0.0337
6	0	6	6	6	←	5	1	5	5	5	20827.6928	0.0306
6	0	6	7	7	←	5	1	5	6	6	20827.7174	0.0056
6	0	6	6	7	←	5	1	5	5	6	20827.7861	-0.0238
6	0	6	5	4	←	5	1	5	4	3	20828.0077	-0.0434
2	2	1	3	2	←	1	1	0	2	1	20908.9834	0.0209
2	2	1	2	1	←	1	1	0	0	1	20909.4565	0.0004
2	2	1	3	3	←	1	1	0	2	3	20909.9753	0.0227
2	2	1	1	2	←	1	1	0	0	1	20910.4856	0.0110
2	2	1	2	3	←	1	1	0	2	2	20910.9556	-0.0987
2	2	1	3	4	←	1	1	0	2	3	20910.9556	0.0946
2	2	1	2	2	←	1	1	0	1	1	20911.3482	-0.0010
2	2	1	3	3	←	1	1	0	1	2	20911.8129	0.0100
2	2	0	3	3	←	1	1	1	1	2	21549.1346	-0.0054
2	2	0	2	3	←	1	1	1	2	2	21550.3361	-0.0251
2	2	0	3	4	←	1	1	1	2	3	21551.1374	0.0008
2	2	0	1	2	←	1	1	1	2	1	21551.6676	0.0068
2	2	0	3	2	←	1	1	1	0	1	21552.7449	-0.0200
3	3	1	3	4	←	3	2	2	4	4	22068.9123	-0.0498
3	3	1	3	2	←	3	2	2	3	4	22069.5263	-0.0185
3	3	1	4	5	←	3	2	2	3	2	22070.1122	0.0812
6	1	6	5	4	←	3	2	2	4	4	22070.1122	-0.0223
6	1	6	7	8	←	5	0	5	4	3	23349.8766	0.0417
6	1	6	7	6	←	5	0	5	6	7	23349.8766	-0.0089
6	1	6	6	7	←	5	0	5	6	5	23349.8766	0.0183
6	1	6	6	5	←	5	0	5	5	6	23350.2199	-0.0570
3	2	2	4	5	←	5	0	5	5	4	23350.2199	-0.0382
3	2	2	4	4	←	2	1	1	3	4	24318.9586	-0.0060
3	2	2	4	3	←	2	1	1	3	4	24318.9586	-0.0062
3	2	2	3	4	←	2	1	1	3	3	24319.4157	0.0219
3	2	2	4	4	←	2	1	1	3	3	24319.4157	0.0220
3	3	1	4	4	←	2	1	1	2	3	24319.8775	0.0326
3	2	2	3	3	←	2	1	1	2	2	24320.1792	0.0356

Table 19: Assigned transitions of the hydantoin $^{13}\text{C}(5)$ isotopologue in the 18-26 GHz region.

J'	K'_a	K'_c	F'_1	F'_2		J	K_a	K_c	F_1	F_2	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
6	1	6	5	4	←	5	1	5	5	5	18065.6371	-0.0002
6	1	6	7	6	←	5	1	5	6	6	18066.6700	0.0535
6	1	6	5	6	←	5	1	5	4	4	18066.6700	-0.1165
6	1	6	7	8	←	5	1	5	5	6	18067.2588	0.0291
6	1	6	6	6	←	5	1	5	5	4	18067.6176	0.0146
6	1	6	6	5	←	4	0	4	5	6	20642.6163	-0.0108
6	1	6	6	7	←	4	0	4	3	4	20642.6163	0.0450
6	1	6	5	5	←	4	0	4	3	2	20642.6163	0.1076
6	1	6	7	7	←	4	0	4	4	5	20643.2088	0.0742
2	2	0	1	1	←	4	0	4	4	3	20643.2088	0.1317
2	2	0	2	3	←	4	0	4	3	3	20643.2088	-0.0754
2	2	0	3	3	←	4	0	4	5	5	20643.2088	-0.1363
2	2	0	3	3	←	4	0	4	4	4	20643.8911	0.0376
2	2	1	3	4	←	5	1	5	4	5	20750.6500	-0.0366
2	2	1	2	3	←	5	1	5	5	4	20750.6500	-0.0258
2	2	1	1	2	←	5	1	5	6	7	20750.6500	0.0217
2	2	1	3	2	←	1	1	0	2	1	21313.4860	-0.0238
2	2	1	3	3	←	1	1	0	0	1	21315.0661	0.0423
5	1	5	6	7	←	1	1	0	2	3	21315.4462	0.0451
5	1	5	4	5	←	1	1	0	2	2	21315.4462	-0.1358
5	1	5	4	3	←	1	1	0	1	2	21316.3363	0.0161
5	1	5	5	6	←	1	1	1	1	2	21936.2282	-0.0179
5	1	5	5	4	←	1	1	1	2	3	21937.1521	0.0093
5	1	5	4	4	←	1	1	1	2	2	21937.4618	-0.0013
5	1	5	6	6	←	1	1	1	2	2	21938.2618	0.0191
5	1	5	5	5	←	5	0	5	4	3	23523.2882	0.0120
3	2	2	3	4	←	5	0	5	6	5	23523.2882	-0.0146
3	2	2	2	3	←	5	0	5	4	5	23523.2882	-0.0183
3	2	2	2	2	←	5	0	5	6	7	23523.2882	-0.0491
3	2	2	4	3	←	5	0	5	5	4	23523.6911	-0.0129
5	2	4	5	5	←	5	0	5	5	6	23523.6911	-0.0439
5	2	4	6	6	←	5	0	5	4	4	23523.8855	0.0425
5	2	4	4	4	←	5	0	5	6	6	23523.8855	0.0082
5	2	4	5	6	←	5	0	5	5	5	23524.2848	0.0043
5	2	4	5	4	←	2	1	1	1	2	24731.8534	-0.0854
6	0	6	5	6	←	2	1	1	1	1	24731.8534	-0.0686
6	0	6	6	5	←	2	1	1	3	2	24731.8534	0.0872
6	0	6	7	8	←	2	1	1	3	3	24732.5676	0.0091

H. Coordinates of Heavy Atoms in Hydantoin from the r_s Structure Analysis

Table 20: The coordinates of the heavy atoms in hydantoin obtained from the r_s structure.

atom	x	y	z
¹⁵ N(1)	0.00000	-0.92840	0.0000
¹³ C(2)	1.14552	-0.14371	0.0000
¹⁵ N(3)	0.73892	1.15269	0.0000
¹³ C(4)	-0.70014	1.28530	0.0000
¹³ C(5)	-1.16887	-0.15687	0.0000

References

- [1] H. M. Pickett. The fitting and prediction of vibration-rotation spectra with spin interactions. *Journal of Molecular Spectroscopy*, 148(2):371–377, 1991.
- [2] D. Christen, J.H. Griffiths, and J. Sheridan. The microwave spectrum of imidazole; complete structure and the electron distribution from nuclear quadrupole coupling tensors and dipole moment orientation. *Zeitschrift für Naturforschung A*, 36(12):1378–1385, 1982.
- [3] Z. Kisiel. PROSPE - Programs for Rotational Spectroscopy, 2015.
- [4] S. Gruet, C. Pérez, A.L. Steber, and M. Schnell. Where's water? The many binding sites of hydantoin. *Physical Chemistry Chemical Physics*, 20:5545–5552, 2018.