

Chirped-pulse Fourier transform millimeter-wave
spectroscopy of ten vibrationally excited states of
i-propyl cyanide: Exploring the far-infrared region
- Supplementary Material -

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Table 1: Quantum-chemical vs. experimentally determined rotational constants for the ground state and the ten vibrationally excited states of *i*-propyl cyanide. To support the assignment of the vibrationally excited states, the calculated rotational constants were shifted by 94.80 MHz for A, 7.95 MHz for B, and 22.72 MHz for C, which is the difference between experimental and calculated rotational constants determined for the ground state.

Molecule	Rotational	A (MHz)	B (MHz)	C (MHz)
State	Constants			
Ground	Ab initio	7846.08	3960.14	2878.35
State	Experimental	7940.8746(16)	3968.08888(52)	2901.05458(53)
ν_{30}	Ab initio	7804.35	3972.04	2876.90
	Experimental	7896.7463(15)	3980.03092(59)	2899.86118(61)
ν_{29}	Ab initio	7840.05	3957.50	2875.94
	Experimental	7932.486(46)	3964.9549(50)	2898.2120(45)
ν_{17}	Ab initio	7891.83	3963.23	2881.13
	Experimental	7994.048(20)	3971.8740(22)	2904.7207(14)
ν_{16}	Ab initio	7831.30	3962.36	2880.74
	Experimental	7923.1764(24)	3970.27231(63)	2902.82671(69)
ν_{15}	Ab initio	7836.46	3970.84	2878.19
	Experimental	7928.435(15)	3978.7235(14)	2900.5124(14)
$2\nu_{30}$	Ab initio	7762.62	3983.94	2875.46
	Experimental	7853.1241(69)	3991.94840(76)	2898.60041(73)
$(\nu_{30}+\nu_{29})$	Ab initio	7798.32	3969.40	2874.50
	Experimental	7879.481(28)	3976.7219(54)	2896.9396(33)
$(\nu_{30}+\nu_{17})$	Ab initio	7850.09	3975.13	2879.69
	Experimental	7945.628(27)	3983.3608(56)	2903.4154(23)
$(\nu_{29}+\nu_{17})$	Ab initio	7885.80	3960.59	2878.73
	Experimental	-	-	-
$2\nu_{29}$	Ab initio	7834.03	3954.86	2873.54
	Experimental	7926.817(25)	3963.9296(49)	2896.3754(36)
$2\nu_{17}$	Ab initio	7937.57	3966.34	2883.91
	Experimental	-	-	-
$(\nu_{30}+\nu_{16})$	Ab initio	7789.60	3974.26	2879.33
	Experimental	7875.091(21)	3981.9721(22)	2901.5706(16)

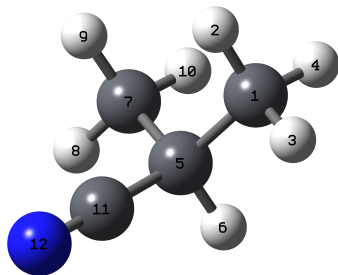


Figure 1: Structure of *i*-propyl cyanide and labeling of carbon atoms for comparison with the atomic coordinates reported in Table 3.

Table 2: Experimentally determined atom positions (following the Kraitchman procedure) for the four carbon atoms as labeled in Figure 1.

Atom Number	Element	x	y	z
1	C	-1.123	1.272	0.151
5	C	-0.463	0	-0.402
7	C	-1.123	-1.272	0.151
11	C	0.967	0	-0.108

Table 3: Quantum-chemically determined atomic coordinates obtained from the structure optimisation calculation employing the B3LYP/aug-cc-pVTZ level of theory. The labeling follows Figure 1.

Atom Number	Element	x	y	z
1	C	-1.126	1.277	0.154
2	H	-1.047	1.318	1.240
3	H	-0.659	2.170	-0.256
4	H	-2.182	1.285	-0.115
5	C	-0.466	0	-0.391
6	H	-0.559	0	-1.481
7	C	-1.126	-1.277	0.154
8	H	-0.659	-2.170	-0.256
9	H	-1.047	-1.318	1.240
10	H	-2.182	-1.285	-0.115
11	C	0.971	0	-0.101
12	N	2.096	0	0.139

Table 4: Experimentally determined molecular parameters for the ^{13}C isotopologues of *i*-propyl cyanide, following the labeling of Figure 1.

Parameters	$^{13}\text{C}(1)$ and $^{13}\text{C}(7)$	$^{13}\text{C}(11)$	$^{13}\text{C}(5)$
A (MHz)	7747.279(28)	7939.368(33)	7921.780(27)
B (MHz)	3927.9450(53)	3939.1212(53)	3956.5392(56)
C (MHz)	2854.3725(40)	2885.7232(30)	2897.6257(31)
D_J (kHz)	0.6061(64)	0.5914(64)	0.6099(64)
D_{JK} (kHz)	11.739(12)	12.359(37)	11.497(30)
D_K (kHz)	[-5.231]	[-5.231]	[-5.231]
d_1 (kHz)	-0.2460(62)	-0.2455(52)	-0.2318(51)
d_2 (kHz)	-0.1914(22)	-0.1929(21)	-0.1759(21)
No. (lines)	38	31	32
rms (kHz)	41.9	41.2	48.3

Table 5: Experimental linelist for the vibronic ground state of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
26	8	19	←	26	6	20	75376.49219	-0.02716
25	7	19	←	25	5	20	75479.44531	-0.02007
22	4	18	←	22	4	19	76382.09375	-0.01380
12	2	11	←	11	2	10	76574.16406	0.00913
11	2	9	←	10	2	8	76665.48438	-0.01184
12	1	11	←	11	1	10	76693.00781	-0.01685
11	7	4	←	10	7	3	76778.97656	0.01142
22	5	18	←	22	3	19	76780.43750	0.03130
11	4	8	←	10	4	7	77031.63281	-0.00528
11	6	6	←	10	6	5	77099.68750	-0.08481
19	2	17	←	19	2	18	77407.56250	0.01619
19	3	17	←	19	1	18	77419.89062	0.00465
11	5	7	←	10	5	6	77436.71875	0.00871
13	1	13	←	12	1	12	77744.38281	-0.01392
13	0	13	←	12	0	12	77745.84375	-0.02502
27	8	20	←	27	6	21	78042.67188	-0.01510
11	5	6	←	10	5	5	78077.47656	0.04068
24	6	19	←	24	4	20	78342.52344	0.00157
31	8	23	←	31	8	24	78407.61719	0.00458
21	3	18	←	21	3	19	79621.36719	-0.04057
21	4	18	←	21	2	19	79676.89062	-0.00972
26	7	20	←	26	5	21	79824.50781	0.00116
11	4	7	←	10	4	6	80454.64844	-0.00828
12	3	10	←	11	3	9	80869.35156	-0.01573
11	3	8	←	10	3	7	81008.26562	0.00375
23	4	19	←	23	4	20	81366.63281	-0.01581
23	5	19	←	23	3	20	81568.99219	0.02084
29	7	22	←	29	7	23	81603.77344	0.01261
28	8	21	←	28	6	22	81631.89062	-0.01069
28	9	20	←	28	7	21	81637.80469	-0.00217
34	9	25	←	34	9	26	81875.58594	-0.01111

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
20	2	18	←	20	2	19	82098.41406	-0.00446
20	3	18	←	20	1	19	82104.00781	-0.01113
12	2	10	←	11	2	9	82163.62500	-0.01916
13	2	12	←	12	2	11	82393.62500	-0.00827
13	1	12	←	12	1	11	82451.44531	-0.00481
25	5	20	←	25	5	21	82498.53125	0.00814
27	6	21	←	27	6	22	82738.65625	0.01188
25	6	20	←	25	4	21	83129.07031	-0.00196
14	1	14	←	13	1	13	83545.17969	-0.00552
14	0	14	←	13	0	13	83545.71875	-0.08669
12	8	4	←	11	8	3	83660.91406	0.04780
12	4	9	←	11	4	8	83760.28906	0.06814
22	3	19	←	22	3	20	84385.98438	0.04620
22	4	19	←	22	2	20	84412.28125	-0.06906
30	9	22	←	30	7	23	84463.17188	0.05941
27	7	21	←	27	5	22	84467.75781	0.02034
12	6	6	←	11	6	5	84476.21875	0.05536
12	5	8	←	11	5	7	84619.11719	-0.00707
37	10	27	←	37	10	28	84912.67188	-0.01023
29	8	22	←	29	6	23	85839.17188	-0.06277
12	5	7	←	11	5	6	85913.70312	0.00561
32	8	24	←	32	8	25	86091.56250	-0.01329
24	4	20	←	24	4	21	86264.54688	0.00438
24	5	20	←	24	3	21	86365.34375	0.00246
21	2	19	←	21	2	20	86780.37500	0.03439
21	3	19	←	21	1	20	86782.81250	-0.04160
13	3	11	←	12	3	10	86876.44531	0.02084
12	3	9	←	11	3	8	87618.33594	-0.01045
26	5	21	←	26	5	22	87640.53125	0.00338
13	2	11	←	12	2	10	87664.64062	0.00113
31	9	23	←	31	7	24	87727.14062	0.03231
26	6	21	←	26	4	22	87969.20312	0.00385
30	7	23	←	30	7	24	88000.83594	-0.02850
14	2	13	←	13	2	12	88201.13281	-0.01501

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
14	1	13	←	13	1	12	88228.46875	0.00798
28	6	22	←	28	6	23	88331.78906	-0.02175
12	4	8	←	11	4	7	88512.46094	-0.00710
5	4	2	←	4	2	3	89127.00781	0.02421
23	4	20	←	23	2	21	89139.39062	0.00925
28	7	22	←	28	5	23	89275.88281	-0.02355
15	0	15	←	14	0	14	89345.96094	0.00456
32	10	23	←	32	8	24	89359.75000	-0.01068
31	10	22	←	31	8	23	89495.81250	0.00983
35	9	26	←	35	9	27	90205.82812	0.00923
13	4	10	←	12	4	9	90310.61719	0.00643
30	8	23	←	30	6	24	90432.17188	0.01362
33	10	24	←	33	8	25	90929.24219	-0.00102
25	4	21	←	25	4	22	91106.72656	0.05006
13	7	7	←	12	7	6	91156.64844	0.00358
22	2	20	←	22	2	21	91455.50781	-0.05822
13	6	8	←	12	6	7	91618.90625	-0.01795
13	5	9	←	12	5	8	91729.06250	0.00037
32	9	24	←	32	7	25	91751.10938	-0.01545
13	6	7	←	12	6	6	91941.09375	0.02342
27	5	22	←	27	5	23	92657.20312	0.02672
14	3	12	←	13	3	11	92796.25781	0.01886
14	2	12	←	13	2	11	93241.48438	-0.02346
21	2	20	←	21	0	21	93396.17969	-0.02423
21	1	20	←	21	1	21	93396.17969	0.04143
13	3	10	←	12	3	9	93707.25781	-0.01354
34	10	25	←	34	8	26	93800.58594	0.05140
24	3	21	←	24	3	22	93851.42969	0.01224
31	7	24	←	31	7	25	93891.13281	0.03185
15	2	14	←	14	2	13	94002.88281	0.00848
15	1	14	←	14	1	13	94015.48438	-0.00081
13	5	8	←	12	5	7	94035.32031	0.01674
29	7	23	←	29	5	24	94163.57812	0.00827
16	1	16	←	15	1	15	95146.05469	0.04265

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
31	8	24	←	31	6	25	95246.58594	0.00100
26	4	22	←	26	4	23	95911.34375	-0.06474
26	5	22	←	26	3	23	95935.18750	-0.05416
23	2	21	←	23	2	22	96125.55469	0.03038
23	3	21	←	23	1	22	96126.02344	0.00714
13	4	9	←	12	4	8	96260.77344	0.00467
33	9	25	←	33	7	26	96262.53125	-0.01234
35	11	25	←	35	9	26	96583.14062	-0.04975
14	4	11	←	13	4	10	96680.10156	0.00675
24	9	16	←	24	7	17	97373.43750	-0.03546
36	11	26	←	36	9	27	97480.14844	-0.01296
36	9	27	←	36	9	28	97578.54688	0.00349
28	6	23	←	28	4	24	97676.87500	0.05616
22	2	21	←	22	0	22	98041.35156	-0.04441
14	7	8	←	13	7	7	98420.78906	0.02585
14	7	7	←	13	7	6	98483.37500	0.01387
25	3	22	←	25	3	23	98563.44531	0.04016
15	3	13	←	14	3	12	98658.21094	-0.02571
14	5	10	←	13	5	9	98719.85156	0.00094
30	6	24	←	30	6	25	98816.51562	0.01256
15	2	13	←	14	2	12	98896.35156	-0.01165
14	6	9	←	13	6	8	98908.07812	0.00293
30	7	24	←	30	5	25	99079.48438	-0.02978
14	3	11	←	13	3	10	99360.19531	0.00090
32	7	25	←	32	7	26	99436.59375	-0.01622
14	6	8	←	13	6	7	99603.58594	-0.01565
16	2	15	←	15	2	14	99802.03906	-0.01198
16	1	15	←	15	1	14	99807.76562	0.00351
37	11	27	←	37	9	28	99886.19531	0.01657
32	8	25	←	32	6	26	100174.13281	-0.01946
27	4	23	←	27	4	24	100689.73438	0.00862
27	5	23	←	27	3	24	100701.10938	0.03695
17	0	17	←	16	0	16	100946.18750	-0.00916
17	1	17	←	16	1	16	100946.19531	0.03557

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
39	10	29	←	39	10	30	101884.89844	-0.01668
36	10	27	←	36	8	28	101983.55469	0.01905
14	5	9	←	13	5	8	102343.00000	-0.01287
29	5	24	←	29	5	25	102473.13281	-0.00561
29	6	24	←	29	4	25	102514.85938	0.01344
23	2	22	←	23	0	23	102685.35156	-0.01362
15	4	12	←	14	4	11	102882.70312	-0.00614
26	3	23	←	26	3	24	103265.62500	0.00696
26	4	23	←	26	2	24	103266.82812	0.01511
14	4	10	←	13	4	9	103552.10156	-0.02788
31	7	25	←	31	5	26	103995.36719	0.00248
39	12	28	←	39	10	29	104153.37500	0.00666
37	9	28	←	37	9	29	104199.55469	0.05623
16	3	14	←	15	3	13	104485.32812	-0.00156
18	8	11	←	18	6	12	104604.02344	0.03568
16	2	14	←	15	2	13	104607.57031	-0.00745
33	7	26	←	33	7	27	104754.74219	0.03745
15	3	12	←	14	3	11	104774.76562	0.04593
35	8	27	←	35	8	28	104976.28125	0.00183
33	8	26	←	33	6	27	105147.70312	-0.05912
15	8	8	←	14	8	7	105205.82031	0.02881
15	8	7	←	14	8	6	105216.17188	0.02397
15	5	11	←	14	5	10	105552.25000	-0.00937
17	1	16	←	16	1	15	105602.77344	0.00970
15	7	9	←	14	7	8	105731.21094	-0.01049
15	7	8	←	14	7	7	105885.81250	0.00845
40	12	29	←	40	10	30	106017.20312	-0.00657
15	6	10	←	14	6	9	106174.03125	-0.01748
32	11	22	←	32	9	23	106223.07031	0.01616
18	0	18	←	17	0	17	106746.14062	-0.00324
18	1	18	←	17	1	17	106746.14062	0.01453
37	10	28	←	37	8	29	106747.25000	-0.03619
30	5	25	←	30	5	26	107315.32031	-0.04849
24	2	23	←	24	0	24	107328.27344	0.00771

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
30	6	25	←	30	4	26	107335.71875	0.00144
15	6	9	←	14	6	8	107530.33594	0.00084
39	11	29	←	39	9	30	107618.52344	0.01663
27	3	24	←	27	3	25	107959.86719	0.01020
27	4	24	←	27	2	25	107960.42969	0.03251
32	6	26	←	32	6	27	108828.65625	-0.03625
32	7	26	←	32	5	27	108896.92188	0.01574
16	4	13	←	15	4	12	108945.14062	-0.06475

Table 6: Experimental linelist for ν_{30} of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
20	3	17	←	20	3	18	75161.93750	0.02859
20	4	17	←	20	2	18	75257.47656	0.04509
25	7	19	←	25	5	20	75857.71875	0.01342
12	2	11	←	11	2	10	76561.82031	-0.03196
11	9	2	←	10	9	1	76563.19531	0.01882
11	2	9	←	10	2	8	76626.42188	-0.00779
12	1	11	←	11	1	10	76669.55469	-0.00413
11	8	3	←	10	8	2	76716.41406	0.01592
22	4	18	←	22	4	19	76851.80469	0.00316
11	4	8	←	10	4	7	77154.34375	-0.02601
22	5	18	←	22	3	19	77182.67969	-0.07744
11	6	5	←	10	6	4	77330.22656	0.07796
11	5	7	←	10	5	6	77608.94531	-0.00153
19	2	17	←	19	2	18	77661.88281	0.04313
13	1	13	←	12	1	12	77717.65625	-0.02864
13	0	13	←	12	0	12	77718.95312	-0.02310
24	5	19	←	24	5	20	77832.09375	0.03444
24	5	19	←	24	5	20	77832.09375	0.03444
11	5	6	←	10	5	5	78311.85156	-0.00770
24	6	19	←	24	4	20	78814.07031	-0.03115
21	3	18	←	21	3	19	79959.99219	-0.03404
21	4	18	←	21	2	19	80005.70312	0.06359
26	7	20	←	26	5	21	80315.85938	0.00164
11	4	7	←	10	4	6	80743.97656	-0.00831
12	3	10	←	11	3	9	80895.80469	-0.02581
11	3	8	←	10	3	7	81136.21094	-0.01677
23	4	19	←	23	4	20	81817.75781	-0.02358
23	5	19	←	23	3	20	81983.60156	-0.02543
28	8	21	←	28	6	22	82025.65625	-0.00770
12	2	10	←	11	2	9	82111.54688	-0.00863
20	3	18	←	20	1	19	82363.48438	0.04191
13	2	12	←	12	2	11	82376.92188	-0.01079

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
13	1	12	←	12	1	11	82428.57812	-0.04572
25	5	20	←	25	5	21	83113.02344	-0.06374
12	11	2	←	11	11	1	83388.06250	0.04902
12	10	2	←	11	10	1	83494.50781	-0.01404
14	1	14	←	13	1	13	83516.09375	0.01300
14	0	14	←	13	0	13	83516.61719	-0.00075
12	9	3	←	11	9	2	83637.07031	0.05570
12	8	4	←	11	8	3	83836.42969	-0.04949
12	4	9	←	11	4	8	83870.10938	-0.00885
12	7	5	←	11	7	4	84136.59375	0.04906
12	6	7	←	11	6	6	84537.67188	0.01506
12	6	6	←	11	6	5	84689.28906	-0.00499
12	5	8	←	11	5	7	84800.42188	-0.00233
9	6	4	←	9	4	5	84850.60938	-0.01702
27	7	21	←	27	5	22	85029.39062	-0.04123
12	5	7	←	11	5	6	86209.70312	-0.01879
35	13	23	←	35	12	23	86784.83594	-0.01914
24	5	20	←	24	3	21	86787.68750	-0.08979
13	3	11	←	12	3	10	86888.65625	0.00467
21	3	19	←	21	1	20	87049.62500	0.05682
13	2	11	←	12	2	10	87615.60938	0.00942
12	3	9	←	11	3	8	87685.56250	0.01974
14	2	13	←	13	2	12	88180.96875	-0.00526
14	1	13	←	13	1	12	88205.08594	0.01018
26	6	21	←	26	4	22	88485.50000	-0.00010
12	4	8	←	11	4	7	88798.35938	-0.00757
28	6	22	←	28	6	23	89116.24219	0.06166
23	3	20	←	23	3	21	89470.75000	-0.04099
23	4	20	←	23	2	21	89480.64062	-0.07236
28	7	22	←	28	5	23	89878.47656	-0.04915
13	12	2	←	12	12	1	90321.50781	0.00244
13	4	10	←	12	4	9	90401.78906	-0.02679
13	11	3	←	12	11	2	90425.42188	-0.02910
13	10	3	←	12	10	2	90560.17188	0.02313

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
13	9	4	←	12	9	3	90741.25781	0.01465
13	8	5	←	12	8	4	90996.77344	0.05662
13	7	7	←	12	7	6	91365.35156	0.07075
13	7	6	←	12	7	5	91391.88281	0.00059
13	6	8	←	12	6	7	91835.20312	-0.01760
13	5	9	←	12	5	8	91911.00000	-0.00884
13	6	7	←	12	6	6	92197.28125	0.01172
32	9	24	←	32	7	25	92345.59375	0.06577
14	2	12	←	13	2	11	93200.76562	0.00839
13	3	10	←	12	3	9	93705.58594	0.01040
15	2	14	←	14	2	13	93979.80469	0.00606
15	1	14	←	14	1	13	93990.77344	-0.00699
29	6	23	←	29	6	24	94387.59375	-0.02101
13	5	8	←	12	5	7	94394.21875	-0.00817
16	0	16	←	15	0	15	95112.21094	-0.04378
9	4	6	←	8	3	6	95173.75781	-0.04357
31	8	24	←	31	6	25	95953.57812	-0.02175
13	4	9	←	12	4	8	96510.68750	-0.01119
14	4	11	←	13	4	10	96749.22656	-0.00847
14	11	3	←	13	11	2	97484.39062	0.00803
14	10	4	←	13	10	3	97652.26562	0.05990
14	9	5	←	13	9	4	97879.01562	-0.00152
14	8	7	←	13	8	6	98198.46875	0.02848
22	2	21	←	22	0	22	98269.49219	0.05200
15	3	13	←	14	3	12	98650.06250	-0.03753
14	7	8	←	13	7	7	98653.63281	-0.03166
14	7	7	←	13	7	6	98725.92188	-0.02442
15	2	13	←	14	2	12	98862.82031	0.00114
14	5	10	←	13	5	9	98892.89844	-0.03461
14	6	9	←	13	6	8	99140.53906	-0.03250
14	3	11	←	13	3	10	99303.53125	0.01130
16	2	15	←	15	2	14	99776.39062	0.01337
16	1	15	←	15	1	14	99781.26562	-0.02621
14	6	8	←	13	6	7	99917.59375	-0.03156

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
32	7	25	←	32	7	26	100333.42969	0.01123
17	0	17	←	16	0	16	100910.00781	0.01797
17	1	17	←	16	1	16	100910.00781	0.05435
14	5	9	←	13	5	8	102741.57812	-0.02482
23	1	22	←	23	1	23	102921.67188	0.00773
15	4	12	←	14	4	11	102929.29688	-0.01172
14	4	10	←	13	4	9	103739.23438	0.03662
15	12	4	←	14	12	3	104408.72656	-0.04605
16	3	14	←	15	3	13	104470.78125	-0.05194
15	11	4	←	14	11	3	104566.67969	0.00528
16	2	14	←	15	2	13	104578.48438	0.00383
15	3	12	←	14	3	11	104693.75000	0.01655
15	10	5	←	14	10	4	104773.16406	0.04268
15	9	7	←	14	9	6	105053.32812	0.01233
15	9	6	←	14	9	5	105053.92188	0.05221
27	13	15	←	27	12	15	105401.72656	0.03760
15	8	8	←	14	8	7	105448.73438	-0.01329
15	8	7	←	14	8	6	105461.00781	-0.01074
17	2	16	←	16	2	15	105572.13281	0.01607
17	1	16	←	16	1	15	105574.28125	0.00406
15	5	11	←	14	5	10	105707.40625	0.01813
15	7	9	←	14	7	8	105988.33594	-0.01305
7	7	1	←	6	6	1	106123.69531	0.04801
15	7	8	←	14	7	7	106166.21094	-0.00452
15	6	10	←	14	6	9	106415.50781	-0.00881
18	0	18	←	17	0	17	106707.61719	0.02890
15	6	9	←	14	6	8	107917.51562	0.01219
16	4	13	←	15	4	12	108971.31250	-0.01500

Table 7: Experimental linelist for ν_{17} of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
11	8	4	←	10	8	3	76629.18750	-0.00713
12	2	11	←	11	2	10	76694.51562	0.02728
12	1	11	←	11	1	10	76819.52344	-0.01218
11	2	9	←	10	2	8	76825.34375	0.02574
11	4	8	←	10	4	7	77118.83594	-0.05343
11	6	5	←	10	6	4	77212.00781	0.10748
11	5	7	←	10	5	6	77503.96875	-0.02069
13	1	13	←	12	1	12	77850.98438	-0.02594
13	0	13	←	12	0	12	77852.53125	-0.05039
11	5	6	←	10	5	5	78121.22656	0.01380
11	4	7	←	10	4	6	80485.17188	-0.01287
12	3	10	←	11	3	9	80995.97656	-0.00042
11	3	8	←	10	3	7	81114.38281	0.01710
12	2	10	←	11	2	9	82334.83594	0.02966
13	2	12	←	12	2	11	82522.32812	0.00051
13	1	12	←	12	1	11	82583.53125	-0.00119
14	1	14	←	13	1	13	83659.23438	0.13179
14	0	14	←	13	0	13	83659.67188	-0.09991
12	8	4	←	11	8	3	83734.54688	0.03875
12	4	9	←	11	4	8	83864.59375	-0.02969
12	7	6	←	11	7	5	84013.62500	0.05798
12	7	5	←	11	7	4	84020.62500	-0.01075
12	6	7	←	11	6	6	84410.68750	-0.07509
12	6	6	←	11	6	5	84538.44531	-0.09125
12	5	8	←	11	5	7	84696.04688	-0.01361
12	5	7	←	11	5	6	85947.42188	0.00260
13	3	11	←	12	3	10	87017.02344	-0.01914
12	3	9	←	11	3	8	87762.64844	0.01769
13	2	11	←	12	2	10	87839.35156	0.04030
14	2	13	←	13	2	12	88337.67969	0.00987
14	1	13	←	13	1	12	88366.76562	-0.00103
12	4	8	←	11	4	7	88562.27344	-0.01348

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
15	1	15	←	14	1	14	89466.96094	0.06890
13	4	10	←	12	4	9	90433.88281	-0.00989
13	7	7	←	12	7	6	91231.42188	-0.00190
13	7	6	←	12	7	5	91252.96875	-0.04676
13	6	8	←	12	6	7	91692.97656	-0.02041
13	5	9	←	12	5	8	91818.96094	-0.01955
13	6	7	←	12	6	6	91999.90625	0.02355
14	3	12	←	13	3	11	92949.14844	-0.02433
14	2	12	←	13	2	11	93417.25781	0.00001
13	3	10	←	12	3	9	93891.13281	-0.04379
13	5	8	←	12	5	7	94059.23438	0.04020
15	2	14	←	14	2	13	94146.93750	0.01688
15	1	14	←	14	1	13	94160.45312	0.02193
16	1	16	←	15	1	15	95274.48438	0.01210
16	0	16	←	15	0	15	95274.48438	-0.10390
13	4	9	←	12	4	8	96343.24219	0.02464
14	4	11	←	13	4	10	96822.82812	-0.02287
14	7	8	←	13	7	7	98498.85156	-0.02980
14	7	7	←	13	7	6	98557.84375	0.06349
15	3	13	←	14	3	12	98821.80469	-0.01928
14	5	10	←	13	5	9	98826.28125	-0.09247
14	6	9	←	13	6	8	98989.09375	-0.00145
15	2	13	←	14	2	12	99073.92969	0.01895
14	3	11	←	13	3	10	99575.93750	0.00022
14	6	8	←	13	6	7	99653.46094	0.02377
16	2	15	←	15	2	14	99953.45312	0.03409
16	1	15	←	15	1	14	99959.59375	0.01980
17	1	17	←	16	1	16	101081.84375	-0.02969
17	0	17	←	16	0	16	101081.84375	-0.07745
14	5	9	←	13	5	8	102367.58594	0.10645
15	4	12	←	14	4	11	103044.28125	-0.03059
14	4	10	←	13	4	9	103677.09375	0.03834
16	3	14	←	15	3	13	104658.21094	0.01346
16	2	14	←	15	2	13	104788.50781	0.03415

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
15	3	12	←	14	3	11	105007.25000	-0.00490
17	2	16	←	16	2	15	105758.87500	0.05949
17	1	16	←	16	1	15	105761.59375	0.01740
15	7	8	←	14	7	7	105958.57031	0.02775
18	1	18	←	17	1	17	106889.04688	-0.03506
15	6	9	←	14	6	8	107565.43750	-0.09521
16	4	13	←	15	4	12	109123.94531	-0.03900

Table 8: Experimental linelist for ν_{29} of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
12	2	11	←	11	2	10	76501.90625	0.00449
11	2	9	←	10	2	8	76593.31250	0.02450
12	1	11	←	11	1	10	76620.26562	0.03806
11	6	6	←	10	6	5	77036.35156	0.09536
11	6	5	←	10	6	4	77086.37500	-0.02940
11	5	7	←	10	5	6	77372.53906	-0.00972
13	1	13	←	12	1	12	77669.51562	-0.01370
13	0	13	←	12	0	12	77670.87500	-0.11880
11	4	7	←	10	4	6	80392.46094	0.00187
12	3	10	←	11	3	9	80795.50000	0.02277
11	3	8	←	10	3	7	80939.35156	0.00167
12	2	10	←	11	2	9	82085.67188	0.00410
13	2	12	←	12	2	11	82315.74219	0.01020
13	1	12	←	12	1	11	82373.28906	0.02116
12	6	7	←	11	6	6	84272.64062	0.03782
12	6	6	←	11	6	5	84407.46094	-0.04126
12	5	8	←	11	5	7	84548.77344	-0.02608
12	5	7	←	11	5	6	85846.57812	-0.08240
13	3	11	←	12	3	10	86796.41406	0.03761
12	3	9	←	11	3	8	87541.01562	-0.00400
13	2	11	←	12	2	10	87581.64062	0.06990
14	2	13	←	13	2	12	88117.69531	0.02154
14	1	13	←	13	1	12	88144.87500	0.02666
12	4	8	←	11	4	7	88442.98438	0.05626
15	1	15	←	14	1	14	89259.70312	-0.04183
13	4	10	←	12	4	9	90231.10156	-0.09353
13	6	8	←	12	6	7	91544.03125	0.03946
13	5	9	←	12	5	8	91652.22656	-0.09723
13	6	7	←	12	6	6	91867.32812	-0.01093
14	3	12	←	13	3	11	92710.28906	0.03277
14	2	12	←	13	2	11	93153.63281	0.08704
13	3	10	←	12	3	9	93621.51562	-0.13540

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
13	4	9	←	12	4	8	96182.94531	0.05569
14	4	11	←	13	4	10	96593.97656	-0.01888
15	3	13	←	14	3	12	98566.62500	0.11303
14	5	10	←	13	5	9	98636.40625	-0.04530
14	6	8	←	13	6	7	99525.13281	-0.02534
14	5	9	←	13	5	8	102265.19531	-0.00078
15	4	12	←	14	4	11	102790.03906	-0.05348
14	4	10	←	13	4	9	103465.35156	0.05500
15	5	11	←	14	5	10	105461.92969	-0.09216
17	1	16	←	16	1	15	105502.94531	0.03411
15	6	10	←	14	6	9	106087.16406	0.09751
15	6	9	←	14	6	8	107447.54688	0.05388
16	4	13	←	15	4	12	108846.23438	-0.09838

Table 9: Experimental linelist for ν_{16} of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
22	4	18	←	22	4	19	76316.50000	0.00355
11	10	2	←	10	10	1	76353.41406	0.08009
11	9	3	←	10	9	2	76460.44531	-0.03070
12	2	11	←	11	2	10	76605.41406	0.00079
11	8	3	←	10	8	2	76609.36719	0.02724
11	2	9	←	10	2	8	76674.90625	-0.01947
12	1	11	←	11	1	10	76721.67969	0.00426
11	4	8	←	10	4	7	77073.09375	-0.04235
11	6	6	←	10	6	5	77151.33594	0.06091
11	6	5	←	10	6	4	77202.39844	0.00059
11	5	7	←	10	5	6	77487.24219	0.00552
13	1	13	←	12	1	12	77786.65625	0.06276
13	0	13	←	12	0	12	77788.00781	-0.01808
11	5	6	←	10	5	5	78138.85156	-0.03342
21	4	18	←	21	2	19	79574.83594	0.08502
11	4	7	←	10	4	6	80522.62500	-0.03646
12	3	10	←	11	3	9	80899.50781	-0.00387
11	3	8	←	10	3	7	81042.78906	-0.04489
23	4	19	←	23	4	20	81286.31250	-0.00558
12	2	10	←	11	2	9	82174.89062	0.00051
27	9	19	←	27	7	20	82302.95312	-0.00080
13	1	12	←	12	1	11	82484.42188	0.02518
12	11	2	←	11	11	1	83279.31250	0.00175
12	10	2	←	11	10	1	83383.06250	0.05136
12	9	3	←	11	9	2	83521.50781	-0.03200
14	1	14	←	13	1	13	83591.01562	0.04437
12	8	4	←	11	8	3	83715.15625	-0.04300
12	4	9	←	11	4	8	83801.23438	-0.01497
12	7	5	←	11	7	4	84005.78906	-0.02387
12	6	7	←	11	6	6	84398.73438	-0.01631
12	6	6	←	11	6	5	84536.19531	-0.00139
12	5	8	←	11	5	7	84672.67969	0.00250

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
12	5	7	←	11	5	6	85987.28125	0.00341
24	4	20	←	24	4	21	86171.60938	0.00045
24	4	20	←	24	4	21	86171.60938	0.00045
13	3	11	←	12	3	10	86907.26562	0.00400
12	3	9	←	11	3	8	87643.03906	-0.02027
13	2	11	←	12	2	10	87681.07812	0.01050
14	2	13	←	13	2	12	88238.86719	0.02379
14	1	13	←	13	1	12	88265.42969	0.01175
12	4	8	←	11	4	7	88579.35938	-0.02758
15	0	15	←	14	0	14	89395.20312	-0.12034
15	1	15	←	14	1	14	89395.20312	0.12952
13	12	2	←	12	12	1	90203.71094	-0.03334
13	4	10	←	12	4	9	90350.34375	-0.00552
13	10	3	←	12	10	2	90436.08594	0.00265
35	9	26	←	35	9	27	90442.65625	0.04720
13	9	4	←	12	9	3	90612.10156	0.05749
25	4	21	←	25	4	22	91002.42969	-0.03009
13	7	7	←	12	7	6	91218.13281	0.05420
13	7	6	←	12	7	5	91241.71094	0.00864
13	6	8	←	12	6	7	91680.92188	-0.04011
13	5	9	←	12	5	8	91784.10938	-0.00052
16	11	6	←	16	10	6	92620.60156	-0.05273
14	3	12	←	13	3	11	92828.50000	0.01258
14	2	12	←	13	2	11	93264.13281	-0.00287
13	3	10	←	12	3	9	93721.36719	-0.03097
15	2	14	←	14	2	13	94044.06250	0.01913
15	1	14	←	14	1	13	94056.28125	-0.00232
13	5	8	←	12	5	7	94120.83594	-0.04034
16	1	16	←	15	1	15	95199.00781	0.01293
26	4	22	←	26	4	23	95796.69531	-0.02220
23	2	21	←	23	2	22	95978.42188	0.00203
23	2	21	←	23	2	22	95978.42188	0.00203
13	4	9	←	12	4	8	96320.61719	0.00017
14	4	11	←	13	4	10	96718.22656	0.00821

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
14	13	2	←	13	13	1	97126.35156	-0.06257
14	12	3	←	13	12	2	97226.00000	-0.04552
14	11	3	←	13	11	2	97351.50781	-0.07726
14	10	4	←	13	10	3	97514.83594	0.06807
14	9	5	←	13	9	4	97735.05469	0.03547
14	7	8	←	13	7	7	98487.99219	-0.04815
14	5	10	←	13	5	9	98774.71875	-0.00679
15	2	13	←	14	2	12	98924.85938	0.00467
14	6	9	←	13	6	8	98974.30469	-0.04747
23	12	12	←	23	11	12	99114.76562	0.04683
14	3	11	←	13	3	10	99367.20312	-0.01022
32	13	20	←	32	12	20	99635.92969	0.01213
14	6	8	←	13	6	7	99684.35938	-0.02482
16	2	15	←	15	2	14	99846.78906	0.02461
16	1	15	←	15	1	14	99852.26562	-0.02574
24	2	22	←	24	2	23	100635.54688	0.00304
17	0	17	←	16	0	16	101002.75781	-0.04014
17	1	17	←	16	1	16	101002.75781	0.00186
14	5	9	←	13	5	8	102435.81250	0.01597
23	2	22	←	23	0	23	102514.85938	-0.00314
15	4	12	←	14	4	11	102919.46094	0.01799
14	4	10	←	13	4	9	103600.37500	-0.00660
15	14	2	←	14	14	1	104047.11719	0.01412
15	13	3	←	14	13	2	104145.66406	-0.01671
15	12	3	←	14	12	2	104267.13281	0.01348
15	11	4	←	14	11	3	104420.84375	0.05986
16	3	14	←	15	3	13	104522.37500	-0.00408
15	10	5	←	14	10	4	104621.46875	0.06420
16	2	14	←	15	2	13	104641.24219	-0.02042
15	3	12	←	14	3	11	104781.27344	0.03624
15	9	6	←	14	9	5	104893.67188	-0.17793
15	9	7	←	14	9	6	104893.67188	0.29713
15	8	7	←	14	8	6	105287.75000	-0.02252
15	5	11	←	14	5	10	105605.47656	0.03285

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
17	2	16	←	16	2	15	105648.53125	0.00647
17	1	16	←	16	1	15	105650.92188	-0.06278
15	7	9	←	14	7	8	105804.24219	-0.02459
15	7	8	←	14	7	7	105963.04688	0.02688
15	6	10	←	14	6	9	106243.18750	0.00557
37	10	28	←	37	8	29	106702.30469	-0.05710
18	0	18	←	17	0	17	106806.32031	-0.04885
16	4	13	←	15	4	12	108981.26562	0.03673
40	10	30	←	40	10	31	109085.82812	-0.00003

Table 10: Experimental linelist for ν_{15} of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
11	10	2	←	10	10	1	76435.73438	0.04568
11	10	1	←	10	10	0	76435.73438	0.04567
11	9	2	←	10	9	1	76544.99219	0.01324
11	9	3	←	10	9	2	76544.99219	0.01418
12	2	11	←	11	2	10	76591.39844	-0.00345
11	2	9	←	10	2	8	76683.10156	-0.02398
11	8	4	←	10	8	3	76696.75781	-0.01048
12	1	11	←	11	1	10	76703.62500	-0.00414
11	7	5	←	10	7	4	76918.76562	-0.06972
11	4	8	←	10	4	7	77149.81250	-0.01004
11	6	5	←	10	6	4	77303.11719	0.01583
11	5	7	←	10	5	6	77586.24219	0.05299
13	1	13	←	12	1	12	77739.74219	0.02762
13	0	13	←	12	0	12	77741.10156	0.02282
11	5	6	←	10	5	5	78266.55469	0.02524
12	3	10	←	11	3	9	80923.04688	-0.00696
11	3	8	←	10	3	7	81141.85938	-0.01092
12	2	10	←	11	2	9	82172.40625	-0.01808
13	2	12	←	12	2	11	82408.60938	0.00557
13	1	12	←	12	1	11	82462.74219	0.00202
12	10	3	←	11	10	2	83474.59375	-0.02606
14	1	14	←	13	1	13	83539.49219	0.07340
14	0	14	←	13	0	13	83539.91406	-0.07666
12	9	3	←	11	9	2	83615.96875	0.03689
12	8	4	←	11	8	3	83813.46875	-0.04888
12	4	9	←	11	4	8	83873.67969	0.01699
12	7	6	←	11	7	5	84102.08594	0.07699
12	6	7	←	11	6	6	84509.16406	0.00777
12	6	6	←	11	6	5	84654.28906	-0.03844
12	5	8	←	11	5	7	84778.69531	0.03184
12	5	7	←	11	5	6	86146.83594	-0.00451
13	3	11	←	12	3	10	86922.28906	-0.00729

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
13	2	11	←	12	2	10	87674.63281	-0.00484
12	3	9	←	11	3	8	87717.48438	0.00296
14	2	13	←	13	2	12	88214.35156	-0.02088
14	1	13	←	13	1	12	88239.71875	-0.02608
12	4	8	←	11	4	7	88748.32812	-0.00533
15	0	15	←	14	0	14	89339.03906	-0.05009
13	11	2	←	12	11	1	90403.65625	-0.07631
13	4	10	←	12	4	9	90415.17188	0.00807
13	10	3	←	12	10	2	90537.42969	0.00854
13	9	4	←	12	9	3	90716.99219	0.06058
13	8	5	←	12	8	4	90969.82812	-0.04325
13	7	7	←	12	7	6	91335.00000	0.01482
13	7	6	←	12	7	5	91360.20312	0.00281
13	6	8	←	12	6	7	91803.52344	-0.02476
13	5	9	←	12	5	8	91893.29688	-0.01382
13	6	7	←	12	6	6	92150.71875	-0.01570
14	3	12	←	13	3	11	92835.64844	0.00102
14	2	12	←	13	2	11	93256.30469	-0.00743
13	3	10	←	12	3	9	93765.10938	-0.02200
15	2	14	←	14	2	13	94014.69531	-0.00241
15	1	14	←	14	1	13	94026.32031	0.00318
13	5	8	←	12	5	7	94314.42969	-0.01365
31	7	24	←	31	7	25	94767.13281	0.00176
16	0	16	←	15	0	15	95138.19531	-0.00436
13	4	9	←	12	4	8	96480.97656	-0.00189
14	4	11	←	13	4	10	96773.14062	0.01734
14	13	2	←	13	13	1	97230.27344	0.07718
14	11	3	←	13	11	2	97459.88281	-0.01100
14	10	4	←	13	10	3	97626.38281	0.01982
14	9	5	←	13	9	4	97851.07812	-0.01287
14	7	8	←	13	7	7	98618.59375	-0.02038
15	3	13	←	14	3	12	98692.81250	0.05535
15	2	13	←	14	2	12	98915.63281	0.01156
14	6	9	←	13	6	8	99107.44531	0.00459

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
14	3	11	←	13	3	10	99383.70312	0.04131
16	2	15	←	15	2	14	99812.67188	0.01285
16	1	15	←	15	1	14	99817.89844	0.01756
14	6	8	←	13	6	7	99854.34375	-0.00556
17	0	17	←	16	0	16	100937.25000	0.01385
14	5	9	←	13	5	8	102654.89062	0.01884
15	4	12	←	14	4	11	102963.37500	0.00369
15	12	4	←	14	12	3	104382.32031	-0.07625
16	3	14	←	15	3	13	104516.35938	0.01183
15	11	4	←	14	11	3	104539.14844	0.00109
16	2	14	←	15	2	13	104629.75000	-0.00297
15	10	5	←	14	10	4	104743.86719	0.03679
17	2	16	←	16	2	15	105609.66406	-0.05692
17	1	16	←	16	1	15	105612.02344	-0.00419
15	5	11	←	14	5	10	105707.40625	-0.07682
15	7	9	←	14	7	8	105948.64062	-0.08835
15	7	8	←	14	7	7	106117.81250	0.03979
40	12	29	←	40	10	30	106345.25781	-0.00057
15	6	10	←	14	6	9	106383.71875	0.01834
18	0	18	←	17	0	17	106736.14844	0.02445
15	6	9	←	14	6	8	107832.46875	0.03094
16	4	13	←	15	4	12	109014.36719	0.03636

Table 11: Experimental linelist for $2\nu_{30}$ of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
12	2	11	←	11	2	10	76547.40625	0.01729
11	2	9	←	10	2	8	76583.05469	-0.01888
11	10	2	←	10	10	1	76600.57031	0.04430
12	1	11	←	11	1	10	76644.82031	-0.01274
11	8	3	←	10	8	2	76872.66406	0.00544
11	4	8	←	10	4	7	77273.82031	-0.03340
11	6	5	←	10	6	4	77511.89844	0.06580
13	1	13	←	12	1	12	77689.21875	-0.01739
13	0	13	←	12	0	12	77690.37500	0.00718
11	5	6	←	10	5	5	78550.60156	-0.00305
21	3	18	←	21	3	19	80289.90625	-0.00447
21	4	18	←	21	2	19	80327.33594	0.01662
12	3	10	←	11	3	9	80918.46875	-0.00953
11	4	7	←	10	4	6	81031.75000	-0.04553
12	2	10	←	11	2	9	82057.70312	0.00684
13	2	12	←	12	2	11	82358.12500	0.02050
13	1	12	←	12	1	11	82404.24219	0.00369
14	1	14	←	13	1	13	83485.09375	-0.02659
14	0	14	←	13	0	13	83485.64844	0.06430
12	11	2	←	11	11	1	83548.89062	0.00146
12	9	3	←	11	9	2	83805.93750	0.00864
12	4	9	←	11	4	8	83975.64844	0.01044
12	8	4	←	11	8	3	84012.28125	-0.06165
29	7	22	←	29	7	23	84103.81250	-0.00357
12	6	6	←	11	6	5	84904.92188	0.08453
12	5	8	←	11	5	7	84979.89062	-0.00691
22	3	19	←	22	3	20	85058.06250	0.03909
22	4	19	←	22	2	20	85075.32812	-0.04463
12	5	7	←	11	5	6	86511.43750	-0.02546
13	3	11	←	12	3	10	86897.17188	-0.00049
13	2	11	←	12	2	10	87566.07031	-0.00601
12	3	9	←	11	3	8	87741.27344	-0.00984

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
14	2	13	←	13	2	12	88158.64844	-0.01214
14	1	13	←	13	1	12	88179.89062	0.00151
12	4	8	←	11	4	7	89077.96094	-0.01103
13	4	10	←	12	4	9	90487.71875	0.02298
13	11	3	←	12	11	2	90602.89062	-0.04163
13	10	4	←	12	10	3	90741.91406	-0.04469
13	9	4	←	12	9	3	90929.24219	0.06594
13	8	6	←	12	8	5	91192.39062	-0.00596
13	8	5	←	12	8	4	91193.86719	0.06005
13	6	8	←	12	6	7	92051.47656	0.01178
13	5	9	←	12	5	8	92089.66406	-0.00877
13	6	7	←	12	6	6	92457.85156	0.00075
14	3	12	←	13	3	11	92794.01562	-0.00890
14	2	12	←	13	2	11	93159.56250	-0.01318
13	3	10	←	12	3	9	93692.33594	0.00109
15	2	14	←	14	2	13	93954.53125	0.00649
15	1	14	←	14	1	13	93964.01562	-0.06198
24	3	21	←	24	3	22	94540.30469	0.05673
24	4	21	←	24	2	22	94543.76562	-0.06353
13	5	8	←	12	5	7	94757.42188	-0.01951
16	0	16	←	15	0	15	95076.30469	-0.03561
14	4	11	←	13	4	10	96812.48438	-0.00197
14	12	3	←	13	12	2	97546.26562	-0.06222
14	11	4	←	13	11	3	97679.26562	-0.00212
14	10	4	←	13	10	3	97852.65625	0.05499
14	9	5	←	13	9	4	98087.23438	-0.03682
14	8	7	←	13	8	6	98418.07031	0.04673
14	8	6	←	13	8	5	98422.78906	-0.03791
15	3	13	←	14	3	12	98638.78125	0.01525
15	2	13	←	14	2	12	98828.39844	0.01542
14	7	8	←	13	7	7	98887.38281	-0.04266
14	5	10	←	13	5	9	99061.04688	-0.00282
14	3	11	←	13	3	10	99238.92969	0.01586
14	6	9	←	13	6	8	99372.03906	-0.05129

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
16	2	15	←	15	2	14	99748.44531	0.00863
16	1	15	←	15	1	14	99752.64844	-0.01211
17	0	17	←	16	0	16	100871.62500	-0.00229
17	1	17	←	16	1	16	100871.62500	0.02796
15	4	12	←	14	4	11	102969.87500	-0.02890
14	5	9	←	13	5	8	103138.75000	0.01122
14	4	10	←	13	4	9	103911.07031	0.02051
16	3	14	←	15	3	13	104453.37500	0.01699
16	2	14	←	15	2	13	104547.95312	0.01083
38	11	28	←	38	9	29	104712.84375	0.00144
15	11	4	←	14	11	3	104779.85156	0.03306
15	10	5	←	14	10	4	104993.24219	0.03442
17	2	16	←	16	2	15	105541.67969	0.01670
17	1	16	←	16	1	15	105543.48438	-0.01131
15	8	8	←	14	8	7	105692.64844	-0.08789
15	5	11	←	14	5	10	105855.89062	-0.00169
25	3	23	←	25	1	24	106040.43750	0.00111
15	7	9	←	14	7	8	106246.22656	0.03884
15	7	8	←	14	7	7	106450.61719	0.02166
15	6	10	←	14	6	9	106654.45312	0.00690
18	0	18	←	17	0	17	106666.78125	-0.00286
15	6	9	←	14	6	8	108313.96094	0.02940
16	4	13	←	15	4	12	108991.74219	0.00414

Table 12: Experimental linelist for $\nu_{30} + \nu_{29}$ of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
11	2	9	←	10	2	8	76537.37500	0.06949
12	1	11	←	11	1	10	76587.67969	-0.09975
11	4	8	←	10	4	7	77083.74219	-0.07738
11	5	7	←	10	5	6	77543.84375	0.04282
13	0	13	←	12	0	12	77640.00000	0.03061
11	5	6	←	10	5	5	78253.10156	-0.04284
11	4	7	←	10	4	6	80686.57812	-0.08094
12	3	10	←	11	3	9	80811.98438	-0.08756
11	3	8	←	10	3	7	81058.31250	-0.00115
12	2	10	←	11	2	9	82016.35156	0.08558
13	2	12	←	12	2	11	82290.65625	-0.04448
13	1	12	←	12	1	11	82341.59375	-0.00656
14	1	14	←	13	1	13	83431.35156	-0.07033
14	0	14	←	13	0	13	83431.90625	-0.03958
12	8	5	←	11	8	4	83766.17188	-0.04046
12	4	9	←	11	4	8	83790.76562	-0.03812
12	5	8	←	11	5	7	84728.26562	0.05328
12	5	7	←	11	5	6	86149.02344	0.04167
13	3	11	←	12	3	10	86797.45312	-0.01844
12	3	9	←	11	3	8	87593.40625	0.05310
14	2	13	←	13	2	12	88089.10156	0.12640
15	0	15	←	14	0	14	89224.24219	0.11381
13	4	10	←	12	4	9	90313.38281	-0.03725
13	7	6	←	12	7	5	91317.30469	0.06428
13	5	9	←	12	5	8	91830.95312	0.09261
13	3	10	←	12	3	9	93599.37500	-0.01068
13	5	8	←	12	5	7	94330.89062	0.07304
16	0	16	←	15	0	15	95016.35938	0.01605
14	4	11	←	13	4	10	96651.66406	-0.12329
14	7	8	←	13	7	7	98573.32812	0.07371
14	7	7	←	13	7	6	98646.64844	0.01526
14	3	11	←	13	3	10	99186.07812	-0.04643

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
16	1	15	←	15	1	14	99677.96094	0.02977
15	4	12	←	14	4	11	102823.10156	-0.04042
16	3	14	←	15	3	13	104360.42969	0.13991
17	1	16	←	16	1	15	105465.35938	-0.06496
15	7	9	←	14	7	8	105902.39062	-0.05707
15	7	8	←	14	7	7	106082.84375	-0.07686
18	0	18	←	17	0	17	106600.52344	-0.02302
18	1	18	←	17	1	17	106600.52344	-0.00876
16	4	13	←	15	4	12	108857.03906	0.00791
16	4	13	←	15	4	12	108857.03906	0.00791

Table 13: Experimental linelist for $\nu_{30} + \nu_{17}$ of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
11	3	9	←	10	3	8	74890.14062	-0.06419
12	2	11	←	11	2	10	76676.21875	0.00487
11	2	9	←	10	2	8	76777.68750	0.04061
11	8	4	←	10	8	3	76778.97656	0.00241
12	1	11	←	11	1	10	76789.38281	0.02834
11	7	5	←	10	7	4	77001.44531	0.12875
11	7	4	←	10	7	3	77003.69531	0.03655
11	4	8	←	10	4	7	77235.68750	-0.05429
11	6	6	←	10	6	5	77331.91406	0.02504
11	6	5	←	10	6	4	77385.69531	0.02287
13	1	13	←	12	1	12	77820.31250	0.03509
13	0	13	←	12	0	12	77821.65625	0.00554
11	5	6	←	10	5	5	78348.34375	0.04135
11	4	7	←	10	4	6	80769.51562	-0.01290
12	3	10	←	11	3	9	81015.60938	-0.00477
11	3	8	←	10	3	7	81236.91406	-0.02002
12	2	10	←	11	2	9	82272.55469	-0.00560
13	2	12	←	12	2	11	82499.32031	0.00609
13	1	12	←	12	1	11	82553.95312	0.02007
14	1	14	←	13	1	13	83625.85156	0.09133
14	0	14	←	13	0	13	83626.25000	-0.08838
12	4	9	←	11	4	8	83968.12500	0.01847
12	7	6	←	11	7	5	84191.94531	-0.00940
12	7	5	←	11	7	4	84200.16406	-0.00650
12	6	7	←	11	6	6	84599.64062	-0.01996
12	6	6	←	11	6	5	84744.17969	0.02919
12	5	8	←	11	5	7	84870.78906	-0.07026
12	5	7	←	11	5	6	86235.45312	0.01892
13	3	11	←	12	3	10	87021.71094	-0.03064
13	2	11	←	12	2	10	87779.47656	0.03474
12	3	9	←	11	3	8	87823.57812	0.00407
14	2	13	←	13	2	12	88310.92969	0.04152

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
14	1	13	←	13	1	12	88336.53125	0.01712
12	4	8	←	11	4	7	88843.84375	0.01252
15	0	15	←	14	0	14	89431.07812	-0.13089
13	4	10	←	12	4	9	90518.03125	0.00373
13	8	5	←	12	8	4	91066.69531	-0.14310
13	7	6	←	12	7	5	91457.34375	-0.12715
13	6	8	←	12	6	7	91901.82812	-0.05927
13	5	9	←	12	5	8	91994.05469	-0.06486
13	6	7	←	12	6	6	92247.49219	-0.02418
14	3	12	←	13	3	11	92941.57031	-0.02066
14	2	12	←	13	2	11	93365.66406	-0.00466
13	3	10	←	12	3	9	93881.53125	0.08985
15	2	14	←	14	2	13	94116.98438	0.01914
15	1	14	←	14	1	13	94128.72656	0.01655
13	5	8	←	12	5	7	94410.50000	0.01913
16	1	16	←	15	1	15	95236.00000	0.01212
16	0	16	←	15	0	15	95236.00000	-0.08544
13	4	9	←	12	4	8	96588.75000	-0.01066
14	4	11	←	13	4	10	96884.15625	0.01885
14	8	7	←	13	8	6	98271.78906	0.10328
14	8	6	←	13	8	5	98275.51562	0.05146
15	3	13	←	14	3	12	98804.82031	-0.06025
15	2	13	←	14	2	12	99029.72656	-0.02058
14	3	11	←	13	3	10	99508.27344	-0.01061
16	2	15	←	15	2	14	99920.67969	0.04130
16	1	15	←	15	1	14	99925.96875	0.05361
17	1	17	←	16	1	16	101040.80469	-0.02648
14	5	9	←	13	5	8	102760.26562	0.09246
15	4	12	←	14	4	11	103082.10938	-0.03940
14	4	10	←	13	4	9	103859.18750	-0.04943
16	3	14	←	15	3	13	104634.41406	0.00754
16	2	14	←	15	2	13	104748.92969	0.00255
15	8	7	←	14	8	6	105535.96875	-0.00014
17	2	16	←	16	2	15	105723.38281	0.01097

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
17	1	16	←	16	1	15	105725.74219	0.03294
15	5	11	←	14	5	10	105826.12500	-0.02022
18	1	18	←	17	1	17	106845.52344	0.02699
18	0	18	←	17	0	17	106845.52344	0.01097

Table 14: Experimental linelist for $2\nu_{29}$ of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
11	2	9	←	10	2	8	76550.39062	0.01190
11	4	8	←	10	4	7	76934.36719	0.05622
13	1	13	←	12	1	12	77621.83594	0.04681
11	5	6	←	10	5	5	77991.39844	0.00748
12	3	10	←	11	3	9	80754.00781	-0.03904
11	3	8	←	10	3	7	80908.07812	-0.00805
12	2	10	←	11	2	9	82038.26562	-0.02792
14	0	14	←	13	0	13	83413.89844	-0.08699
12	4	9	←	11	4	8	83651.73438	0.00240
12	5	8	←	11	5	7	84517.88281	0.04469
12	5	7	←	11	5	6	85823.60938	-0.00411
13	3	11	←	12	3	10	86750.36719	-0.04376
12	3	9	←	11	3	8	87501.86719	0.00825
13	2	11	←	12	2	10	87530.89062	-0.04730
12	4	8	←	11	4	7	88419.30469	-0.00086
15	0	15	←	14	0	14	89205.07812	0.11967
13	4	10	←	12	4	9	90190.48438	-0.00867
13	6	7	←	12	6	6	91837.64062	-0.06647
14	3	12	←	13	3	11	92659.84375	-0.08651
13	3	10	←	12	3	9	93574.03125	0.03182
16	0	16	←	15	0	15	94995.96875	0.00637
13	4	9	←	12	4	8	96153.11719	0.00526
14	4	11	←	13	4	10	96548.14844	-0.00614
15	3	13	←	14	3	12	98512.00000	-0.03394
14	5	10	←	13	5	9	98597.73438	0.02930
14	3	11	←	13	3	10	99212.00000	0.05086
14	6	8	←	13	6	7	99495.94531	0.03873
16	1	15	←	15	1	14	99654.67188	0.10223
17	1	17	←	16	1	16	100786.82031	-0.04658
17	0	17	←	16	0	16	100786.82031	-0.08936
14	5	9	←	13	5	8	102242.25000	-0.05238
15	4	12	←	14	4	11	102739.01562	-0.05642

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
14	4	10	←	13	4	9	103427.48438	0.03785
16	3	14	←	15	3	13	104329.56250	0.00398
17	1	16	←	16	1	15	105440.65625	0.12445
18	1	18	←	17	1	17	106577.66406	-0.07241
15	6	9	←	14	6	8	107419.76562	0.01663
16	4	13	←	15	4	12	108790.21094	-0.03544

Table 15: Experimental linelist for $\nu_{30} + \nu_{16}$ of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
11	2	9	←	10	2	8	76626.42188	0.04350
12	1	11	←	11	1	10	76693.00781	-0.02221
11	8	3	←	10	8	2	76763.00000	0.04094
11	4	8	←	10	4	7	77191.25781	-0.08151
11	5	7	←	10	5	6	77656.81250	0.01932
13	1	13	←	12	1	12	77757.14062	0.07394
13	0	13	←	12	0	12	77758.35156	0.03471
11	5	6	←	10	5	5	78373.35156	0.04875
11	4	7	←	10	4	6	80811.09375	-0.01781
12	3	10	←	11	3	9	80919.40625	-0.02897
11	3	8	←	10	3	7	81163.02344	-0.00197
12	2	10	←	11	2	9	82113.60156	-0.02979
13	2	12	←	12	2	11	82406.13281	-0.00018
13	1	12	←	12	1	11	82456.32812	0.00851
12	11	1	←	11	11	0	83437.38281	-0.01236
14	1	14	←	13	1	13	83558.82812	-0.08225
14	0	14	←	13	0	13	83559.41406	-0.01658
12	4	9	←	11	4	8	83905.46094	0.01854
12	6	7	←	11	6	6	84592.28125	0.01287
12	5	8	←	11	5	7	84850.60938	0.05306
12	5	7	←	11	5	6	86284.39062	-0.00086
13	3	11	←	12	3	10	86912.40625	0.01389
13	2	11	←	12	2	10	87623.39844	0.01506
12	3	9	←	11	3	8	87699.57031	-0.01560
14	2	13	←	13	2	12	88213.37500	0.01799
14	1	13	←	13	1	12	88236.71875	0.03300
12	4	8	←	11	4	7	88862.00000	0.00878
15	0	15	←	14	0	14	89360.67969	-0.04724
13	9	4	←	12	9	3	90796.88281	0.02421
13	7	6	←	12	7	5	91451.64844	-0.06991
13	6	8	←	12	6	7	91894.60156	-0.02075
13	5	9	←	12	5	8	91961.54688	-0.04108

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
14	3	12	←	13	3	11	92821.60156	-0.00936
14	2	12	←	13	2	11	93215.08594	0.00102
15	2	14	←	14	2	13	94015.48438	-0.01958
13	5	8	←	12	5	7	94481.21094	-0.05495
16	0	16	←	15	0	15	95162.01562	-0.00868
13	4	9	←	12	4	8	96564.06250	0.00444
14	4	11	←	13	4	10	96779.28125	0.00457
14	11	4	←	13	11	3	97543.10938	-0.06222
14	10	5	←	13	10	4	97711.80469	-0.01654
14	9	6	←	13	9	5	97939.78906	0.07670
15	3	13	←	14	3	12	98676.67188	0.00413
14	7	8	←	13	7	7	98718.48438	0.04321
14	5	10	←	13	5	9	98942.03125	0.01250
14	6	9	←	13	6	8	99203.68750	0.01019
14	3	11	←	13	3	10	99296.67969	0.02621
16	2	15	←	15	2	14	99815.49219	-0.00078
16	1	15	←	15	1	14	99820.21875	-0.00500
14	6	8	←	13	6	7	99999.18750	0.02779
17	1	17	←	16	1	16	100963.24219	0.03615
17	0	17	←	16	0	16	100963.24219	0.00141
14	5	9	←	13	5	8	102834.45312	-0.00492
15	4	12	←	14	4	11	102956.97656	-0.00164
14	4	10	←	13	4	9	103777.22656	-0.00279
16	3	14	←	15	3	13	104499.87500	-0.01124
16	2	14	←	15	2	13	104604.02344	0.00323
15	3	12	←	14	3	11	104686.87500	-0.04256
15	10	6	←	14	10	5	104837.88281	0.01445
17	2	16	←	16	2	15	105614.69531	0.01186
17	1	16	←	16	1	15	105616.72656	-0.03654
15	5	11	←	14	5	10	105753.25781	-0.00571
15	7	9	←	14	7	8	106058.73438	-0.02492
15	7	8	←	14	7	7	106242.17969	0.02819
15	6	10	←	14	6	9	106480.56250	-0.02409
18	1	18	←	17	1	17	106764.34375	0.03046

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
16	4	13	←	15	4	12	108997.58594	0.04184

Table 16: Experimental line list for the $^{13}\text{C}(1)$ and $^{13}\text{C}(7)$ of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
12	2	11	←	11	2	10	75378.32812	-0.03297
11	10	1	←	10	10	0	75388.00000	-0.01392
11	2	9	←	10	2	8	75425.07812	0.01636
12	1	11	←	11	1	10	75477.11719	0.03357
11	9	3	←	10	9	2	75499.45312	0.05188
11	8	3	←	10	8	2	75654.39062	0.01307
11	4	8	←	10	4	7	76060.92188	-0.00620
13	0	13	←	12	0	12	76504.84375	0.10475
12	3	10	←	11	3	9	79674.79688	-0.00520
11	4	7	←	10	4	6	79717.21875	-0.04553
11	3	8	←	10	3	7	79984.32812	0.01911
12	2	10	←	11	2	9	80817.79688	-0.06905
13	2	12	←	12	2	11	81100.82812	-0.05159
13	1	12	←	12	1	11	81147.75000	-0.04466
14	1	14	←	13	1	13	82210.99219	0.00040
14	0	14	←	13	0	13	82211.48438	0.01951
12	4	9	←	11	4	8	82664.00781	-0.08919
12	5	7	←	11	5	6	85107.83594	0.03751
13	3	11	←	12	3	10	85565.47656	0.00095
13	2	11	←	12	2	10	86240.02344	0.01291
12	3	9	←	11	3	8	86388.50781	0.03000
14	2	13	←	13	2	12	86813.13281	-0.00847
14	1	13	←	13	1	12	86834.76562	-0.04704
15	0	15	←	14	0	14	87918.25000	-0.08608
13	4	10	←	12	4	9	89081.85938	-0.00986
13	9	4	←	12	9	3	89487.10938	0.07005
13	5	9	←	12	5	8	90634.53125	0.02747
13	6	7	←	12	6	6	90973.91406	-0.01322
14	3	12	←	13	3	11	91374.77344	0.03484
14	2	12	←	13	2	11	91745.03906	0.00309
15	2	14	←	14	2	13	92520.67188	0.03560

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J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
15	1	14	←	14	1	13	92530.46094	0.03976
16	0	16	←	15	0	15	93625.21094	0.00979
13	4	9	←	12	4	8	95210.25781	0.00445
14	4	11	←	13	4	10	95315.95312	0.05432
14	11	3	←	13	11	2	96130.92969	-0.04024
14	9	5	←	13	9	4	96530.22656	-0.00050
14	8	6	←	13	8	5	96857.84375	-0.05524

Table 17: Experimental line list for the $^{13}\text{C}(11)$ of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
11	2	9	←	10	2	8	76288.80469	-0.08781
11	6	6	←	10	6	5	76566.70312	0.04354
13	1	13	←	12	1	12	77334.20312	-0.04055
11	4	7	←	10	4	6	79822.23438	-0.06309
12	3	10	←	11	3	9	80418.10938	0.03317
11	3	8	←	10	3	7	80488.97656	0.06938
13	2	12	←	12	2	11	81958.84375	0.01620
13	1	12	←	12	1	11	82021.46094	0.06625
12	7	6	←	11	7	5	83364.68750	0.04028
12	7	5	←	11	7	4	83371.32031	-0.03792
13	3	11	←	12	3	10	86402.67969	-0.02835
13	2	11	←	12	2	10	87235.69531	0.00871
14	2	13	←	13	2	12	87736.56250	-0.01643
14	1	13	←	13	1	12	87766.44531	0.00662
15	1	15	←	14	1	14	88874.35938	0.01940
13	7	6	←	12	7	5	90544.74219	-0.07855
14	3	12	←	13	3	11	92298.61719	0.03608
15	2	14	←	14	2	13	93508.16406	0.01676
15	1	14	←	14	1	13	93522.04688	-0.01834
16	0	16	←	15	0	15	94644.14062	-0.02761
13	4	9	←	12	4	8	95571.63281	0.01941
14	4	11	←	13	4	10	96115.83594	0.02068
14	7	7	←	13	7	6	97788.82031	0.05305
15	3	13	←	14	3	12	98134.77344	-0.00012
15	2	13	←	14	2	12	98392.49219	-0.02520
17	0	17	←	16	0	16	100413.64844	0.01414
15	4	12	←	14	4	11	102301.32031	-0.01631
14	4	10	←	13	4	9	102869.12500	-0.02142
16	2	14	←	15	2	13	104068.15625	0.03952
17	1	16	←	16	1	15	105047.35156	-0.07475
18	1	18	←	17	1	17	106182.99219	0.03152

Table 18: Experimental line list for the $^{13}\text{C}(5)$ of *i*-propyl cyanide.

J'	Ka'	Kc'		J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
13	1	13	←	12	1	12	77642.93750	0.09557
13	0	13	←	12	0	12	77644.36719	0.01056
11	5	6	←	10	5	5	77876.12500	-0.04029
12	3	10	←	11	3	9	80719.15625	-0.09746
11	3	8	←	10	3	7	80813.53906	-0.00043
12	2	10	←	11	2	9	82024.37500	0.03317
14	0	14	←	13	0	13	83437.39062	-0.04371
12	7	6	←	11	7	5	83744.03125	0.04672
13	3	11	←	12	3	10	86721.00781	-0.02861
12	3	9	←	11	3	8	87425.11719	0.03178
14	1	13	←	13	1	12	88095.67188	0.01094
14	3	12	←	13	3	11	92635.36719	-0.09960
14	2	12	←	13	2	11	93087.89062	-0.01026
13	3	10	←	12	3	9	93520.07031	-0.03445
15	1	14	←	14	1	13	93875.71875	0.04826
16	0	16	←	15	0	15	95023.98438	-0.06417
13	4	9	←	12	4	8	96006.89844	0.08518
14	9	5	←	13	9	4	97443.45312	0.02312
15	3	13	←	14	3	12	98491.81250	0.04841
14	5	10	←	13	5	9	98492.58594	-0.00669
16	1	15	←	15	1	14	99661.08594	0.08127
17	0	17	←	16	0	16	100817.27344	-0.00983
14	5	9	←	13	5	8	102049.64062	0.00796
15	4	12	←	14	4	11	102683.21094	-0.03539
14	4	10	←	13	4	9	103296.50781	0.00526
16	3	14	←	15	3	13	104312.83594	0.04467
15	7	9	←	14	7	8	105473.73438	-0.00369
15	7	8	←	14	7	7	105622.83594	-0.07293
18	1	18	←	17	1	17	106610.37500	0.00510
16	4	13	←	15	4	12	108741.61719	0.03829
17	2	16	←	16	2	15	105446.44531	-0.04131
14	4	11	←	13	4	10	96485.06250	-0.02868

Continued on next page

J'	Ka'	Kc'	J	Ka	Kc	Obs. Freq. (MHz)	Obs. - Calc. (MHz)
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References