

Supplementary Information
Rotational spectroscopy of
2,4,6-cycloheptatriene-1-carbonitrile: Facilitating the
search for complex cyclic molecules in the ISM

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S1.0 Experimental details

A brief description of the measurements performed in this work is given as follows: The COMPACT spectrometer Schmitz *et al.* (2012); Pérez *et al.* (2016); Fatima *et al.* (2020) was used to record the spectrum in the 2-8 GHz range. A series of eight chirped pulses covering 2-8 GHz (each of 4 μ s duration) is generated by the arbitrary waveform generator (AWG) and amplified with a 300 W traveling wave tube amplifier. These excitation pulses are then transmitted into the vacuum chamber containing a package of the supersonically expanded, cold molecules, and the interaction between the molecules and the microwave pulses induces a macroscopic polarization of the molecular ensemble. Eight chirped pulses per gas pulse combined with the gas-pulse repetition rate of 8 Hz led to an effective repetition rate of 64 Hz. Following each excitation, the resulting free induction decays (FIDs) of the macroscopic polarization were recorded for 40 μ s. In total, one million FIDs were co-added in the time domain, followed by the fast Fourier transformation into the frequency domain.

The K-band spectrometer, operating in the range of 18-26 GHz Fatima *et al.* (2020), uses the combination of the segmented approach and the multi-train method. The bandwidth of 8 GHz is split into smaller segments of 800 MHz, and the spectrum across the whole bandwidth is obtained by stitching these segments together Neill *et al.* (2013). The multi-train method utilizes multiple pulse trains per molecular gas pulse, increasing the effective repetition rate of the experiment. The AWG synthesizes 1.5 μ s long excitation pulses in the range of 7-3 GHz. These chirps are then frequency upconverted to 9-13 GHz and doubled to 18-26 GHz. For each gas pulse, the molecular ensemble is polarized by a series of three pulse trains. The multi-train setup combined with a gas-pulse repetition

rate of 10 Hz results in an effective repetition rate of 30 Hz. A total of 2.2 million FIDs were collected (each for a duration of 10 μ s), frequency down-converted, co-added, and converted into the frequency domain by fast Fourier transformation.

The W-band spectrometer (75-110 GHz) Arenas *et al.* (2017) also utilizes the segmented approach. The 35 GHz bandwidth is covered in segments of 720 MHz each. Among the different measurement modes available, the high dynamic range (HDR) mode was used for this experiment, which addresses each segment of 720 MHz by 30 chirps of 24 MHz bandwidth, thus reducing the spurious content in the collected spectrum. The AWG synthesizes 500 ns excitation pulses in the 1.5-2.3 GHz range, which is then frequency upconverted and multiplied through a series of mixing stages and an active multiplier chain ($\times 6$) to produce the radiation in the millimeter-wave regime. A total of one million FIDs (each recorded for 4 μ s) were collected followed by conversion into the frequency domain by fast Fourier transformation.

S2.0 Rotational spectra of CHT-1-CN-1 including the nuclear hyperfine splitting patterns for selected transitions.

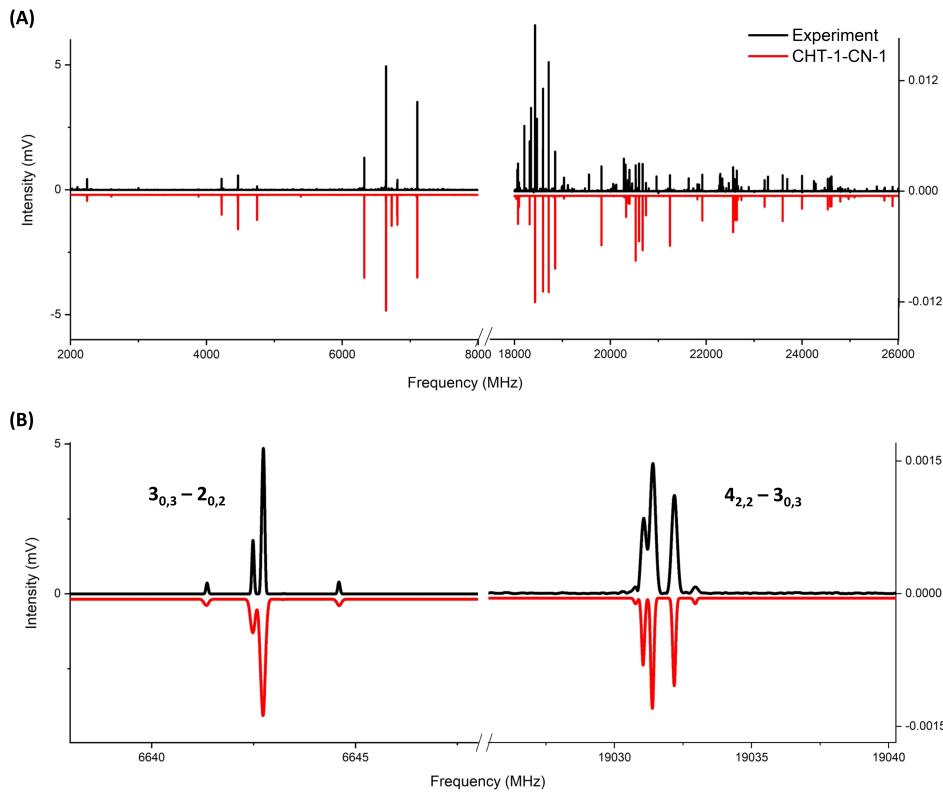


Figure S1: Panel (A) shows the rotational spectra of CHT-1-CN-1 in the frequency range of 2-8, 18-26 GHz. The black trace represents the experimental spectra, and the red trace is the simulated spectra based on the fitted rotational constants at 3 K. Panel (B) shows the zoom-in of the rotational transitions($J_{Ka,Kc} - J'_{Ka',Kc'}$) $3_{0,3} - 2_{0,2}$ and $4_{2,2} - 3_{0,3}$ to highlight the hyperfine splitting observed due to the nuclear quadrupole coupling. To note: the left and right intensity axes correspond to the experiments performed in the different frequency regions.

S3.0 List of rotational transitions of the two conformers in the vibrational ground state.

S3.1 Linelist for CHT-1-CN-1 in the vibrational ground state in 2-26 GHz frequency range

Measured frequencies and residuals (in MHz) for the rotational transitions of CHT-1-CN-1 in 2-26 GHz using SPFIT/SPCAT suite of programs from Pickett.

<i>J</i>	<i>K_a</i>	<i>K_c</i>	<i>F</i>	<i>J'</i>	<i>K'_a</i>	<i>K'_c</i>	<i>F'</i>	Observed	Residuals
								Freq. (MHz)	(MHz)
2	1	2	3	2	0	2	3	2046.851	0.0022
2	1	2	2	2	0	2	2	2047.538	0.0009
7	2	5	7	7	2	6	7	2199.84	-0.0039
7	2	5	8	7	2	6	8	2199.914	0.0042
7	2	5	6	7	2	6	6	2199.914	-0.0053
1	0	1	1	0	0	0	1	2240.953	0.0044
1	0	1	2	0	0	0	1	2242.226	0.0027
1	0	1	0	0	0	0	1	2244.136	-0.0005
1	1	1	2	1	0	1	2	2286.408	-0.0004
1	1	1	0	1	0	1	1	2286.714	0.0046
1	1	1	1	1	0	1	2	2287.058	0.0012
1	1	1	2	1	0	1	1	2287.68	-0.003
1	1	1	1	1	0	1	1	2288.33	-0.0019

8	2	6	8	8	2	7	8	3364.258	-0.0092
8	2	6	7	8	2	7	7	3364.33	-0.0158
8	2	6	9	8	2	7	9	3364.33	-0.0071
2	1	2	2	1	1	1	1	4222.177	0.0022
2	1	2	2	1	1	1	2	4222.829	0.0048
2	1	2	1	1	1	1	1	4223.223	0.0046
2	1	2	3	1	1	1	2	4223.498	0.0035
2	1	2	1	1	1	1	2	4223.867	-0.0003
2	1	2	1	1	1	1	0	4224.844	0.0027
2	0	2	2	1	0	1	2	4461.7	0.0055
2	0	2	1	1	0	1	0	4461.896	0.0001
2	0	2	2	1	0	1	1	4462.971	0.0018
2	0	2	3	1	0	1	2	4463.054	0.0007
2	0	2	1	1	0	1	2	4463.808	-0.0009
2	0	2	1	1	0	1	1	4465.08	-0.0035
2	1	1	2	1	1	0	1	4743.743	0.0036
2	1	1	2	1	1	0	2	4744.37	0.0052
2	1	1	1	1	1	0	1	4744.836	0.0143
2	1	1	3	1	1	0	2	4745.071	0.0114
2	1	1	1	1	1	0	2	4745.446	-0.001
2	1	1	1	1	1	0	0	4746.378	-0.0079
1	1	0	2	0	0	0	1	4789.419	0.0022
1	1	0	1	0	0	0	1	4790.042	-0.0009
9	2	7	9	9	2	8	9	4795.934	-0.0089

9	2	7	10	9	2	8	10	4796.023	0.0116
9	2	7	8	9	2	8	8	4796.023	0.0039
3	1	3	3	2	1	2	3	6321.268	0.017
3	1	3	3	2	1	2	2	6321.943	0.0225
3	1	3	4	2	1	2	3	6322.315	0.0167
3	1	3	2	2	1	2	1	6322.315	0.023
3	1	3	4	2	1	2	3	6322.315	0.0167
3	1	3	2	2	1	2	3	6322.675	0.0096
10	2	8	10	10	2	9	10	6472.015	-0.0009
10	2	8	9	10	2	9	9	6472.096	0.008
10	2	8	11	10	2	9	11	6472.096	0.0146
3	2	2	2	3	1	2	2	6482.057	-0.0309
3	2	2	3	3	1	2	4	6482.457	-0.0063
3	2	2	4	3	1	2	3	6483.528	-0.0085
3	0	3	3	2	0	2	3	6641.355	0.0046
3	0	3	3	2	0	2	3	6641.355	0.0046
3	0	3	2	2	0	2	1	6642.484	0.0014
3	0	3	4	2	0	2	3	6642.737	-0.012
3	0	3	3	2	0	2	2	6642.737	0.0275
3	0	3	2	2	0	2	3	6643.237	-0.0019
3	0	3	2	2	0	2	2	6644.593	-0.0044
3	2	2	3	2	2	1	2	6724.969	0.0098
3	2	2	4	2	2	1	3	6726.314	-0.0109
3	2	2	2	2	2	1	1	6727.075	-0.0099

3	2	1	3	2	2	0	2	6808.279	0.0028
3	2	1	4	2	2	0	3	6809.662	0.0089
3	2	1	2	2	2	0	1	6810.423	0.0083
2	2	1	3	2	1	1	3	6859.719	0.0032
3	1	2	3	2	1	1	3	7102.509	0.0043
3	1	2	3	2	1	1	2	7103.205	0.005
3	1	2	4	2	1	1	3	7103.58	0.0029
3	1	2	2	2	1	1	1	7103.58	0.0141
3	1	2	2	2	1	1	3	7103.957	0.0039
3	1	2	2	2	1	1	2	7104.653	0.0037
2	1	1	1	1	0	1	0	7290.731	0.0029
2	1	1	2	1	0	1	2	7291.556	-0.0028
2	1	1	3	1	0	1	2	7292.254	0
2	1	1	2	1	0	1	1	7292.831	-0.0025
2	1	1	1	1	0	1	1	7293.914	-0.0018
2	2	0	1	2	1	2	1	7661.994	-0.0037
2	2	0	3	2	1	2	3	7663.12	-0.0058
2	2	0	2	2	1	2	2	7665.145	-0.01
4	1	4	4	3	1	3	4	8406.226	0.0074
4	1	4	4	3	1	3	3	8407.267	0.0011
4	1	4	5	3	1	3	4	8407.429	-0.0028
4	1	4	3	3	1	3	2	8407.429	0.052
4	1	4	3	3	1	3	3	8408.784	-0.0076
4	0	4	4	3	0	3	4	8763.869	0.0011

4	0	4	3	3	0	3	2	8765.162	0.0026
4	0	4	5	3	0	3	4	8765.292	0.0075
4	0	4	4	3	0	3	3	8765.292	0.0261
4	0	4	3	3	0	3	3	8767.053	0.0059
4	2	3	4	3	2	2	3	8951.203	0.0067
4	2	3	5	3	2	2	4	8951.78	0.005
4	2	3	3	3	2	2	2	8951.927	0.0038
4	3	2	4	3	3	1	3	9006.149	-0.0012
4	3	2	5	3	3	1	4	9007.413	-0.0035
4	3	2	3	3	3	1	2	9007.903	-0.004
4	3	1	4	3	3	0	3	9012.524	0.0022
4	3	1	5	3	3	0	4	9013.788	-0.0022
4	3	1	3	3	3	0	2	9014.277	-0.0041
4	2	2	4	3	2	1	3	9153.91	-0.0046
4	2	2	5	3	2	1	4	9154.496	-0.0102
4	2	2	3	3	2	1	2	9154.653	-0.0038
4	1	3	4	3	1	2	3	9444.033	0.0126
4	1	3	3	3	1	2	2	9444.182	0.0546
4	1	3	5	3	1	2	4	9444.182	-0.0027
8	7	1	8	7	7	0	7	18000.83	-0.0416
8	7	2	8	7	7	1	7	18000.83	-0.0415
8	7	2	9	7	7	1	8	18001.73	-0.0135
8	7	1	9	7	7	0	8	18001.73	-0.0135
8	6	2	8	7	6	1	7	18015.01	-0.0511

8	6	3	8	7	6	2	7	18015.01	-0.0464
8	6	3	9	7	6	2	8	18015.64	-0.0583
8	6	2	9	7	6	1	8	18015.64	-0.063
8	5	4	8	7	5	3	7	18038.74	-0.0361
8	5	4	8	7	5	3	8	18039.31	0.0299
8	5	4	7	7	5	3	6	18039.31	0.0193
8	5	3	7	7	5	2	6	18039.64	-0.0163
8	5	3	8	7	5	2	8	18039.64	-0.0057
8	5	3	9	7	5	2	8	18039.64	0.0507
8	3	6	8	7	3	5	8	18072.7	-0.0128
8	3	6	9	7	3	5	8	18073.64	-0.0292
8	3	6	7	7	3	5	6	18073.64	-0.0357
8	3	6	7	7	3	5	7	18074.54	-0.0366
8	4	5	8	7	4	4	7	18077.83	-0.015
8	4	5	9	7	4	4	8	18078.15	0.0131
8	4	5	7	7	4	4	6	18078.15	-0.0194
8	4	4	8	7	4	3	7	18092.2	-0.0099
8	4	4	9	7	4	3	8	18092.52	0.0175
8	4	4	7	7	4	3	6	18092.52	-0.0152
4	3	2	3	4	1	3	3	18143.01	-0.004
4	3	2	5	4	1	3	5	18143.46	0.0029
4	3	2	4	4	1	3	4	18145.2	-0.0052
8	3	5	8	7	3	4	8	18314.82	0.0314
8	3	5	9	7	3	4	8	18315.74	-0.0219

8	3	5	7	7	3	4	6	18315.74	-0.0294
8	3	5	7	7	3	4	7	18316.69	0.0029
8	1	7	8	7	1	6	8	18428.67	0.0092
8	1	7	8	7	1	6	7	18430.09	0.0215
8	1	7	7	7	1	6	6	18430.09	0.0312
8	1	7	7	7	1	6	7	18431.68	0.0225
3	3	1	2	3	1	2	2	18579.26	0.0214
3	3	1	4	3	1	2	4	18580.24	0.0086
3	3	1	3	3	1	2	3	18583.05	-0.0171
9	1	9	9	8	1	8	9	18594.71	0.028
9	1	9	10	8	1	8	9	18596.12	-0.0016
9	1	9	9	8	1	8	8	18596.12	0.0156
9	1	9	8	8	1	8	7	18596.12	0.0165
9	1	9	8	8	1	8	8	18597.69	0.0043
9	0	9	9	8	0	8	9	18710.98	0.0049
9	0	9	8	8	0	8	7	18712.43	0.0336
9	0	9	10	8	0	8	9	18712.43	0.0139
9	0	9	9	8	0	8	8	18712.43	0.02
9	0	9	8	8	0	8	8	18714.04	0.0245
3	3	0	4	2	2	0	3	18804.13	0.0306
3	3	0	3	2	2	0	2	18804.51	0.0031
3	3	1	2	2	2	1	2	18822.08	-0.0296
3	3	1	4	2	2	1	3	18824.12	0.0318
3	3	1	3	2	2	1	2	18824.51	0.0152

3	3	1	3	2	2	1	3	18825.85	-0.0107
8	2	6	8	7	2	5	8	18847.18	0.0075
8	2	6	9	7	2	5	8	18848.5	0.0177
8	2	6	7	7	2	5	7	18849.89	0.0175
4	2	2	4	3	0	3	4	19030.75	-0.022
4	2	2	3	3	0	3	2	19031.06	0.0123
4	2	2	5	3	0	3	4	19031.4	0.0102
4	2	2	4	3	0	3	3	19032.18	0.0085
4	2	2	3	3	0	3	3	19032.95	0.0067
5	2	4	6	4	1	4	5	19753.77	-0.0171
5	2	4	5	4	1	4	4	19754.12	0.0043
9	2	8	10	8	2	7	9	19812.11	-0.0318
9	2	8	9	8	2	7	8	19812.11	0.0202
9	2	8	8	8	2	7	7	19812.11	-0.02
9	6	4	9	8	6	3	8	20282.51	-0.0179
9	6	3	9	8	6	2	8	20282.51	-0.0398
9	6	3	8	8	6	2	9	20283.02	0.051
9	6	4	8	8	6	3	7	20283.02	-0.0214
9	6	3	10	8	6	2	9	20283.02	0.018
9	6	3	8	8	6	2	7	20283.02	-0.0433
9	6	4	10	8	6	3	9	20283.02	0.0398
9	5	5	9	8	5	4	8	20316	-0.0179
9	5	5	10	8	5	4	9	20316.34	0.0042
9	5	5	8	8	5	4	8	20316.34	0.0296

9	5	5	8	8	5	4	7	20316.34	-0.0321
9	5	5	8	8	5	4	9	20316.34	-0.0254
9	5	4	9	8	5	3	8	20317.2	-0.0059
9	5	4	10	8	5	3	9	20317.54	0.0126
9	5	4	8	8	5	3	8	20317.54	0.0379
9	5	4	8	8	5	3	7	20317.54	-0.0238
9	5	4	8	8	5	3	9	20317.54	-0.017
9	3	7	9	8	3	6	8	20328.92	-0.071
9	3	7	8	8	3	6	7	20329.13	0.0232
9	3	7	10	8	3	6	9	20329.13	0.0228
9	4	6	8	8	4	5	7	20366.29	-0.047
9	4	6	10	8	4	5	9	20366.29	-0.0312
9	4	5	9	8	4	4	9	20399.39	-0.0313
9	4	5	9	8	4	4	8	20399.92	-0.019
9	4	5	10	8	4	4	9	20400.11	-0.0397
9	4	5	8	8	4	4	7	20400.11	-0.0556
9	1	8	8	8	1	7	7	20527.7	-0.0148
9	1	8	10	8	1	7	9	20527.7	-0.0343
9	1	8	9	8	1	7	8	20527.7	-0.0287
10	1	10	10	9	1	9	10	20595.25	-0.0356
10	1	10	11	9	1	9	10	20596.69	-0.0419
10	1	10	9	9	1	9	8	20596.69	-0.0271
10	1	10	10	9	1	9	9	20596.69	-0.0289
10	1	10	9	9	1	9	9	20598.3	-0.0133

10	0	10	10	9	0	9	9	20672.39	-0.0327
10	0	10	9	9	0	9	8	20672.39	-0.0237
10	0	10	11	9	0	9	10	20672.39	-0.0393
9	3	6	8	8	3	5	7	20743.25	-0.0499
9	3	6	9	8	3	5	8	20743.25	0.0798
9	3	6	10	8	3	5	9	20743.25	-0.0493
4	3	1	3	4	1	4	3	20750.83	-0.0105
4	3	1	5	4	1	4	5	20751.26	-0.0286
4	3	1	4	4	1	4	4	20752.98	-0.015
4	3	1	5	3	2	1	4	21008.25	0.0151
4	3	1	5	3	2	1	4	21008.25	0.0151
4	3	1	4	3	2	1	4	21008.75	0.016
4	3	1	4	3	2	1	3	21008.75	-0.0023
4	3	1	4	3	2	1	3	21008.75	-0.0023
4	3	1	4	3	2	1	4	21008.75	0.016
4	3	2	3	3	2	2	4	21105.05	-0.0069
4	3	2	3	3	2	2	2	21105.05	-0.0064
4	3	2	3	3	2	2	3	21105.05	-0.0068
4	3	2	5	3	2	2	4	21105.2	0.0221
4	3	2	4	3	2	2	3	21105.7	0.0119
4	3	2	4	3	2	2	4	21105.7	0.0118
4	3	2	4	3	2	2	3	21105.7	0.0119
4	3	2	4	3	2	2	4	21105.7	0.0118
9	2	7	9	8	2	6	8	21243.76	-0.0026

9	2	7	10	8	2	6	9	21243.76	-0.0544
9	2	7	8	8	2	6	7	21243.76	-0.0416
5	3	2	4	5	1	5	4	21568.69	0.0056
5	3	2	6	5	1	5	6	21568.89	-0.0267
5	3	2	5	5	1	5	5	21570.07	0.0149
5	2	3	5	4	0	4	5	21813.37	0.037
5	2	3	6	4	0	4	5	21814.23	-0.0257
5	2	3	5	4	0	4	4	21814.77	0.014
5	2	3	4	4	0	4	4	21815.87	0.0006
10	2	9	10	9	2	8	9	21915.88	0.0136
10	2	9	11	9	2	8	10	21915.88	-0.0236
10	2	9	9	9	2	8	8	21915.88	-0.0127
10	7	3	10	9	7	2	9	22527.89	-0.0408
10	7	4	10	9	7	3	9	22527.89	-0.0397
10	7	3	11	9	7	2	10	22528.36	-0.0179
10	7	4	11	9	7	3	10	22528.36	-0.0168
10	7	4	9	9	7	3	8	22528.36	-0.0728
10	6	4	10	9	6	3	9	22555.43	-0.0864
10	6	5	9	9	6	4	9	22555.43	-0.0448
10	6	5	10	9	6	4	9	22555.43	-0.0048
10	6	4	10	9	6	3	10	22555.77	-0.0368
10	6	4	9	9	6	3	10	22555.77	-0.0768
10	6	5	11	9	6	4	10	22555.77	0.0086
10	6	5	9	9	6	4	10	22555.77	0.0048

10	6	4	11	9	6	3	10	22555.77	-0.073
10	6	5	9	9	6	4	8	22555.77	-0.0282
10	1	9	11	9	1	8	10	22557.41	-0.0365
10	1	9	10	9	1	8	9	22557.41	-0.0359
10	1	9	9	9	1	8	8	22557.41	-0.0205
10	3	8	9	9	3	7	8	22570.28	0.0034
10	3	8	11	9	3	7	10	22570.28	-0.0001
11	1	11	12	10	1	10	11	22590.55	-0.0647
11	1	11	11	10	1	10	10	22590.55	-0.0541
11	1	11	10	10	1	10	9	22590.55	-0.052
10	5	6	10	9	5	5	9	22600.73	-0.0635
10	5	6	11	9	5	5	10	22600.96	-0.0645
10	5	5	10	9	5	4	9	22604.03	-0.0605
10	5	5	11	9	5	4	10	22604.27	-0.0611
11	0	11	12	10	0	10	11	22638.23	-0.0539
11	0	11	11	10	0	10	10	22638.23	-0.0472
11	0	11	10	10	0	10	9	22638.23	-0.0411
10	4	6	11	9	4	5	10	22731.02	-0.0539
10	4	6	9	9	4	5	8	22731.02	-0.0613
10	3	7	11	9	3	6	10	23214	-0.0265
10	3	7	9	9	3	6	8	23214	-0.0237
5	3	3	5	4	2	3	5	23425.25	-0.0181
5	3	3	4	4	2	3	3	23425.25	-0.0555
5	3	3	4	4	2	3	3	23425.25	-0.0555

5	3	3	6	4	2	3	5	23425.46	0.0409
5	3	3	4	4	2	3	5	23425.46	0.0091
5	3	3	6	4	2	3	5	23425.46	0.0409
5	3	3	5	4	2	3	4	23425.85	0.0044
5	3	3	5	4	2	3	4	23425.85	0.0044
10	2	8	11	9	2	7	10	23591.9	-0.0648
10	2	8	10	9	2	7	9	23591.9	-0.031
10	2	8	9	9	2	7	8	23591.9	-0.0528
11	2	10	11	10	2	9	10	23995.94	-0.0347
11	2	10	10	10	2	9	9	23995.94	-0.0522
11	2	10	12	10	2	9	11	23995.94	-0.062
10	2	9	11	9	1	8	10	24440.57	0.0041
10	2	9	9	9	1	8	8	24440.57	0.0293
11	1	10	12	10	1	9	11	24532.22	-0.0254
11	1	10	11	10	1	9	10	24532.22	-0.0265
11	1	10	10	10	1	9	9	24532.22	-0.0122
12	1	12	12	11	1	11	11	24579.76	-0.0317
12	1	12	13	11	1	11	12	24579.76	-0.0401
12	1	12	11	11	1	11	10	24579.76	-0.0297
12	0	12	13	11	0	11	12	24609.04	-0.0403
12	0	12	12	11	0	11	11	24609.04	-0.034
12	0	12	11	11	0	11	10	24609.04	-0.0297
11	3	9	10	10	3	8	9	24792.48	-0.0363
11	3	9	11	10	3	8	10	24792.48	0.0221

11	3	9	12	10	3	8	11	24792.48	-0.0412
11	6	6	11	10	6	5	10	24834.38	-0.0288
11	6	6	10	10	6	5	9	24834.62	-0.0597
11	6	5	11	10	6	4	10	24834.62	-0.0439
11	6	6	12	10	6	5	11	24834.62	-0.0371
11	6	5	12	10	6	4	11	24834.86	-0.0644
11	5	7	11	10	5	6	10	24893.47	-0.0502
11	5	7	10	10	5	6	9	24893.63	-0.0788
11	5	7	12	10	5	6	11	24893.63	-0.0672
11	5	6	12	10	5	5	11	24901.78	-0.0604
11	5	6	10	10	5	5	9	24901.78	-0.0721
11	4	8	12	10	4	7	11	24955.6	-0.0156
11	4	8	10	10	4	7	9	24955.6	-0.0181
6	2	4	7	5	0	5	6	24967.36	0.0372
6	2	4	6	5	0	5	5	24967.64	0.0074
11	4	7	10	10	4	6	9	25092.81	-0.0319
11	4	7	12	10	4	6	11	25092.81	-0.029
11	3	8	12	10	3	7	11	25711.27	-0.0065
11	3	8	10	10	3	7	9	25711.27	-0.0021
11	2	9	12	10	2	8	11	25882.02	-0.0527
11	2	9	11	10	2	8	10	25882.02	-0.0317
11	2	9	10	10	2	8	9	25882.02	-0.0418

S3.2 Linelist for CHT-1-CN-1 in the vibrational ground state in 75-110 GHz frequency range

Measured frequencies and residuals (in MHz) for the rotational transitions of CHT-1-CN-1 in 75-110 GHz using SPFIT/SPCAT suite of programs from Pickett..

J	K_a	K_c	J'	K'_a	K'_c	Observed Freq. (MHz)	Residuals (MHz)
33	12	21	32	12	20	74997.5472	-0.0739
33	12	22	32	12	21	74997.5472	0.0391
35	4	32	34	4	31	75093.8874	-0.0268
35	3	32	34	3	31	75096.9191	-0.0208
33	5	28	32	5	27	75129.5587	0.0235
33	11	23	32	11	22	75183.3175	0.0007
33	11	22	32	11	21	75185.0656	-0.0536
36	2	34	35	2	33	75407.8977	-0.0473
36	3	34	35	3	33	75407.8977	0.0333
33	10	24	32	10	23	75433.0484	0.0125
33	10	23	32	10	22	75455.2403	-0.0134
33	7	27	32	7	26	75562.5755	-0.0273
32	6	26	31	6	25	75615.1514	-0.0276
33	9	25	32	9	24	75737.1682	-0.0422
37	1	36	36	1	35	75745.5403	-0.0417
37	2	36	36	2	35	75745.5403	-0.0405
32	7	25	31	7	24	75807.6801	-0.0317

33	8	26	32	8	25		75920.5881	-0.0168
33	9	24	32	9	23		75936.84	-0.0362
38	1	38	37	1	37		76092.8422	-0.0336
38	1	38	37	1	37		76092.8422	-0.0336
38	0	38	37	0	37		76092.8422	-0.0336
34	6	29	33	6	28		76462.0929	0.0302
34	28	6	33	28	5		76504.1865	0.0763
34	28	7	33	28	6		76504.1865	0.0763
34	26	8	33	26	7		76534.2013	0.0187
34	26	9	33	26	8		76534.2013	0.0187
34	25	10	33	25	9		76551.8069	0.0095
34	25	9	33	25	8		76551.8069	0.0095
34	24	10	33	24	9		76571.5361	0.0016
34	24	11	33	24	10		76571.5361	0.0016
34	23	11	33	23	10		76593.8168	0.035
34	23	12	33	23	11		76593.8168	0.035
34	22	12	33	22	11		76619.0531	0.0336
34	22	13	33	22	12		76619.0531	0.0336
34	21	14	33	21	13		76647.8741	0.0256
34	21	13	33	21	12		76647.8741	0.0256
34	20	14	33	20	13		76681.0183	-0.0104
34	20	15	33	20	14		76681.0183	-0.0104
34	19	16	33	19	15		76719.5508	0.0168
34	19	15	33	19	14		76719.5508	0.0168

34	18	16	33	18	15		76764.6556	0.0245
34	18	17	33	18	16		76764.6556	0.0245
35	5	31	34	5	30		76792.619	0.0017
34	17	18	33	17	17		76818.0119	0.0171
34	17	17	33	17	16		76818.0119	0.0171
35	4	31	34	4	30		76834.5362	0.021
34	16	19	33	16	18		76881.8987	0.0137
34	16	18	33	16	17		76881.8987	0.0137
34	15	20	33	15	19		76959.4344	0.0105
34	15	19	33	15	18		76959.4344	0.0105
33	8	25	32	8	24		77037.873	0.005
34	14	21	33	14	20		77055.0533	-0.0001
34	14	20	33	14	19		77055.0533	-0.0007
36	4	33	35	4	32		77070.8845	-0.043
36	3	33	35	3	32		77072.7321	-0.0303
34	13	21	33	13	20		77175.3039	-0.0394
34	13	22	33	13	21		77175.3039	-0.0272
34	12	23	33	12	22		77330.467	0.1081
34	12	22	33	12	21		77330.467	-0.1178
37	3	35	36	3	34		77387.3512	-0.0069
37	2	35	36	2	34		77387.3512	-0.0535
34	11	24	33	11	23		77535.8333	-0.0075
34	11	23	33	11	22		77539.1232	-0.0562
33	6	27	32	6	26		77643.57	-0.0595

34	10	25	33	10	24		77809.6082	-0.0106
34	10	24	33	10	23		77847.6068	0.0261
39	0	39	38	0	38		78073.3227	-0.016
39	1	39	38	1	38		78073.3227	-0.016
34	8	27	33	8	26		78238.9525	0.004
33	7	26	32	7	25		78358.5604	0.021
34	9	25	33	9	24		78432.0178	0.0072
35	6	30	34	6	29		78472.4949	-0.0034
35	28	7	34	28	6		78764.636	0.0167
35	28	8	34	28	7		78764.636	0.0167
36	5	32	35	5	31		78767.9696	0.0576
36	4	32	35	4	31		78794.7837	0.007
35	26	9	34	26	8		78797.3136	-0.0092
35	26	10	34	26	9		78797.3136	-0.0092
35	25	11	34	25	10		78816.5586	0.0656
35	25	10	34	25	9		78816.5586	0.0656
35	5	30	34	5	29		78834.2679	-0.0044
35	24	11	34	24	10		78838.023	0.0403
35	24	12	34	24	11		78838.023	0.0403
35	23	12	34	23	11		78862.2414	0.0251
35	23	13	34	23	12		78862.2414	0.0251
35	22	14	34	22	13		78889.7679	0.0487
35	22	13	34	22	12		78889.7679	0.0487
35	21	15	34	21	14		78921.1484	-0.0008

35	21	14	34	21	13	78921.1484	-0.0008
35	20	16	34	20	15	78957.3912	0.0521
35	20	15	34	20	14	78957.3912	0.0521
35	19	17	34	19	16	78999.3473	-0.01
35	19	16	34	19	15	78999.3473	-0.01
35	19	16	34	19	15	78999.3473	-0.01
35	19	17	34	19	16	78999.3473	-0.01
35	17	18	34	17	17	79106.9041	0.0088
35	17	19	34	17	18	79106.9041	0.0088
35	16	20	34	16	19	79176.7706	0.0191
35	16	19	34	16	18	79176.7706	0.0191
35	15	21	34	15	20	79261.6128	-0.0064
35	15	20	34	15	19	79261.6128	-0.0065
38	2	36	37	2	35	79366.8665	-0.0729
38	3	36	37	3	35	79366.8665	-0.0461
35	13	23	34	13	22	79498.5638	0.0153
35	13	22	34	13	21	79498.5638	-0.0102
34	6	28	33	6	27	79574.0987	0.0014
35	12	24	34	12	23	79669.4975	0.1877
35	12	23	34	12	22	79669.4975	-0.2526
39	2	38	38	2	37	79706.1955	0.0008
39	1	38	38	1	37	79706.1955	0.0004
34	8	26	33	8	25	79729.6777	-0.0296
35	7	29	34	7	28	79855.0389	-0.0012

35	11	25	34	11	24		79895.9552	-0.0249
35	11	24	34	11	23		79902.021	0.0007
40	1	40	39	1	39		80053.7802	0.0165
40	0	40	39	0	39		80053.7802	0.0165
35	10	26	34	10	25		80193.6467	0.0233
35	10	25	34	10	24		80256.994	0.024
36	6	31	35	6	30		80469.9513	-0.0098
35	9	27	34	9	26		80504.4193	0.0076
35	8	28	34	8	27		80531.8728	-0.012
36	5	31	35	5	30		80721.8634	0.0225
37	5	33	36	5	32		80742.3305	0.0152
37	4	33	36	4	32		80759.4062	0.0304
34	7	27	33	7	26		80815.4213	0.025
35	9	26	34	9	25		80971.504	-0.0227
38	4	35	37	4	34		81025.6327	0.0372
38	3	35	37	3	34		81026.2938	0.0352
36	27	9	35	27	8		81042.9024	0.045
36	27	10	35	27	9		81042.9024	0.045
36	26	10	35	26	9		81061.5633	0.0407
36	26	11	35	26	10		81061.5633	0.0407
36	24	13	35	24	12		81105.7089	0.0229
36	24	12	35	24	11		81105.7089	0.0229
36	23	13	35	23	12		81132.0136	-0.0107
36	23	14	35	23	13		81132.0136	-0.0107

36	22	15	35	22	14		81161.9777	0.0492
36	22	14	35	22	13		81161.9777	0.0492
36	21	15	35	21	14		81196.1066	-0.0108
36	21	16	35	21	15		81196.1066	-0.0108
36	20	16	35	20	15		81235.4789	-0.0225
36	20	17	35	20	16		81235.4789	-0.0225
36	19	18	35	19	17		81281.2406	-0.01
36	19	17	35	19	16		81281.2406	-0.01
36	18	19	35	18	18		81334.9059	0.0157
36	18	18	35	18	17		81334.9059	0.0157
39	3	37	38	3	36		81346.5405	0.0239
39	2	37	38	2	36		81346.5405	0.0086
36	17	19	35	17	18		81398.4739	0.0282
35	6	29	34	6	28		81429.0318	0.0451
36	16	21	35	16	20		81474.6537	-0.0097
36	16	20	35	16	19		81474.6537	-0.0097
36	15	22	35	15	21		81567.3737	0.0091
36	15	21	35	15	20		81567.3737	0.009
36	14	23	35	14	22		81682.0388	-0.0015
36	14	22	35	14	21		81682.0388	-0.0042
40	1	39	39	1	38		81686.4725	0.0047
40	2	39	39	2	38		81686.4725	0.0049
36	13	23	35	13	22		81826.938	-0.0159
36	13	24	35	13	23		81826.938	0.0362

36	7	30	35	7	29		81953.2148	0.0026
41	0	41	40	0	40		82034.1494	0.0010
41	1	41	40	1	40		82034.1494	0.0010
36	11	26	35	11	25		82264.0023	-0.0034
36	11	25	35	11	24		82274.6717	-0.0171
35	8	27	34	8	26		82436.9039	-0.0078
37	6	32	36	6	31		82457.7635	-0.0121
36	10	27	35	10	26		82584.069	-0.0136
37	5	32	36	5	31		82629.9062	0.0016
36	10	26	35	10	25		82687.3135	-0.0262
38	5	34	37	5	33		82716.3755	0.0011
38	4	34	37	4	33		82727.1099	-0.0054
36	8	29	35	8	28		82795.2598	-0.0081
36	9	28	35	9	27		82879.5191	0.038
39	4	36	38	4	35		83003.1979	-0.0629
39	3	36	38	3	35		83003.7281	0.0718
35	7	28	34	7	27		83163.1394	0.0028
36	6	30	35	6	29		83237.8325	0.0055
37	31	6	36	31	5		83243.1961	0.0027
37	30	7	36	30	6		83256.9833	0.0889
37	29	9	36	29	8		83271.9669	0.0749
37	28	10	36	28	9		83288.4717	0.0902
37	27	11	36	27	10		83306.6313	0.0358
37	27	10	36	27	9		83306.6313	0.0358

40	2	38	39	2	37		83326.1804	0.0123
37	25	12	36	25	11		83349.3568	-0.0152
37	25	13	36	25	12		83349.3568	-0.0152
37	24	14	36	24	13		83374.6686	-0.0134
37	24	13	36	24	12		83374.6686	-0.0134
37	23	14	36	23	13		83403.2649	0.0173
37	23	15	36	23	14		83403.2649	0.0173
37	22	15	36	22	14		83435.7061	0.012
37	22	16	36	22	15		83435.7061	0.012
37	21	16	36	21	15		83472.8063	0.0012
37	21	17	36	21	16		83472.8063	0.0012
37	20	18	36	20	17		83515.584	0.0091
37	20	17	36	20	16		83515.584	0.0091
36	9	27	35	9	26		83562.3856	-0.0147
37	19	19	36	19	18		83565.2474	-0.0344
37	18	20	36	18	19		83623.6394	0.0434
37	18	19	36	18	18		83623.6394	0.0434
37	17	21	36	17	20		83692.7255	-0.0141
37	17	20	36	17	19		83692.7255	-0.0141
37	16	21	36	16	20		83775.7391	0.0043
37	16	22	36	16	21		83775.7391	0.0043
37	15	23	36	15	22		83876.8346	0.0307
37	15	22	36	15	21		83876.8346	0.0304
37	14	23	36	14	22		84002.0185	-0.0351

42	0	42	41	0	41		84014.4803	-0.0145
42	1	42	41	1	41		84014.4803	-0.0145
37	7	31	36	7	30		84022.8561	0.0269
37	13	24	36	13	23		84160.6883	-0.0682
37	13	25	36	13	24		84160.6883	0.0358
37	12	26	36	12	25		84366.8223	-0.0358
37	12	25	36	12	24		84368.4273	0.0089
38	6	33	37	6	32		84438.7338	-0.004
38	5	33	37	5	32		84554.5347	0.0047
39	5	35	38	5	34		84690.4289	-0.0054
39	4	35	38	4	34		84697.1527	0.0091
37	10	28	36	10	27		84979.4289	0.0008
40	4	37	39	4	36		84981.1653	0.0346
37	8	30	36	8	29		85025.9966	0.0097
37	6	31	36	6	30		85030.4512	-0.0146
36	8	28	35	8	27		85126.9473	0.0025
37	10	27	36	10	26		85143.8228	-0.0003
37	9	29	36	9	28		85242.4513	-0.0012
41	2	39	40	2	38		85305.8481	0.0117
41	3	39	40	3	38		85305.8481	0.0167
36	7	29	35	7	28		85392.9532	-0.0078
38	32	7	37	32	6		85489.3697	0.021
38	31	7	37	31	6		85502.938	0.0346
38	31	8	37	31	7		85502.938	0.0346

38	30	8	37	30	7		85517.708	0.0213
38	30	9	37	30	8		85517.708	0.0213
38	29	9	37	29	8		85533.8514	-0.0261
38	29	10	37	29	9		85533.8514	-0.0261
38	28	11	37	28	10		85551.6764	-0.0112
38	28	10	37	28	9		85551.6764	-0.0112
38	27	12	37	27	11		85571.3908	0.0212
38	27	11	37	27	10		85571.3908	0.0212
38	26	12	37	26	11		85593.2307	0.0043
38	26	13	37	26	12		85593.2307	0.0043
38	25	14	37	25	13		85617.6166	-0.0076
38	25	13	37	25	12		85617.6166	-0.0076
38	24	14	37	24	13		85645.0304	0.0217
38	24	15	37	24	14		85645.0304	0.0217
42	1	41	41	1	40		85646.9442	0.0121
42	2	41	41	2	40		85646.9442	0.0122
38	23	16	37	23	15		85676.0253	0.0971
38	22	17	37	22	16		85711.1664	0.1037
38	22	16	37	22	15		85711.1664	0.1037
38	21	18	37	21	17		85751.2608	-0.0044
38	21	17	37	21	16		85751.2608	-0.0044
38	20	19	37	20	18		85797.6366	0.0173
38	20	18	37	20	17		85797.6366	0.0173
38	19	20	37	19	19		85851.5029	-0.0172

38	19	19	37	19	18		85851.5029	-0.0172
38	18	20	37	18	19		85914.775	-0.0183
38	18	21	37	18	20		85914.775	-0.0183
38	17	21	37	17	20		85989.8465	-0.0275
38	17	22	37	17	21		85989.8465	-0.0275
43	0	43	42	0	42		85994.8076	0.0089
43	1	43	42	1	42		85994.8076	0.0089
38	7	32	37	7	31		86067.4717	-0.0079
38	16	22	37	16	21		86080.0415	-0.0433
38	16	23	37	16	22		86080.0415	-0.0433
37	9	28	36	9	27		86207.8564	-0.0668
38	14	24	37	14	23		86326.6635	-0.0115
38	14	25	37	14	24		86326.6635	0.0002
39	6	34	38	6	33		86415.1064	0.0231
39	5	34	38	5	33		86491.919	-0.013
38	13	26	37	13	25		86500.1684	0.0876
38	13	25	37	13	24		86500.1684	-0.1152
40	5	36	39	5	35		86664.7027	0.0035
40	4	36	39	4	35		86668.8711	0.0109
38	12	27	37	12	26		86726.1562	0.0039
38	12	26	37	12	25		86728.9661	-0.0282
38	6	32	37	6	31		86830.3486	-0.0163
41	3	38	40	3	37		86959.2526	-0.0716
41	4	38	40	4	37		86959.2526	0.067

38	11	28	37	11	27		87024.187	0.0078
38	11	27	37	11	26		87055.4845	0.0029
38	8	31	37	8	30		87222.1981	0.0139
42	2	40	41	2	39		87285.5269	0
42	3	40	41	3	39		87285.5269	0.0029
38	10	29	37	10	28		87377.3803	0.0059
37	7	30	36	7	29		87502.2782	-0.0044
38	9	30	37	9	29		87588.0706	-0.0026
43	1	42	42	1	41		87627.1277	0.0091
43	2	42	42	2	41		87627.1277	0.0091
38	10	28	37	10	27		87632.883	0.0048
39	32	7	38	32	6		87748.814	-0.0006
39	32	8	38	32	7		87748.814	-0.0006
39	31	8	38	31	7		87763.4137	0.007
39	31	9	38	31	8		87763.4137	0.007
37	8	29	36	8	28		87765.0529	-0.0075
39	30	10	38	30	9		87779.3398	0.0099
39	30	9	38	30	8		87779.3398	0.0099
39	29	10	38	29	9		87796.8347	0.0571
39	29	11	38	29	10		87796.8347	0.0571
39	28	11	38	28	10		87816.0401	0.0607
39	28	12	38	28	11		87816.0401	0.0607
39	27	13	38	27	12		87837.2357	0.0271
39	27	12	38	27	11		87837.2357	0.0271

39	26	13	38	26	12		87860.8263	0.0328
39	26	14	38	26	13		87860.8263	0.0328
39	25	14	38	25	13		87887.1185	-0.0125
39	25	15	38	25	14		87887.1185	-0.0125
39	24	16	38	24	15		87916.6958	-0.0087
39	24	15	38	24	14		87916.6958	-0.0087
39	23	16	38	23	15		87950.1131	0.0045
39	23	17	38	23	16		87950.1131	0.0045
44	0	44	43	0	43		87975.0479	-0.012
44	1	44	43	1	43		87975.0479	-0.012
39	22	17	38	22	16		87988.1006	0.0187
39	22	18	38	22	17		87988.1006	0.0187
39	21	18	38	21	17		88031.5397	-0.0117
39	21	19	38	21	18		88031.5397	-0.0117
39	20	19	38	20	18		88081.7111	0.015
39	20	20	38	20	19		88081.7111	0.015
39	7	33	38	7	32		88091.1402	0.0005
39	18	21	38	18	20		88208.5798	0.0147
39	18	22	38	18	21		88208.5798	0.0147
39	17	22	38	17	21		88289.8813	-0.0674
39	17	23	38	17	22		88289.8813	-0.0674
39	16	23	38	16	22		88387.8554	0.0183
39	16	24	38	16	23		88387.8554	0.0184
40	6	35	39	6	34		88388.4763	-0.0418

40	5	35	39	5	34		88438.9378	0.0149
39	15	25	38	15	24		88507.3686	-0.0089
39	15	24	38	15	23		88507.3686	-0.0101
41	5	37	40	5	36		88639.2882	0.0098
41	4	37	40	4	36		88641.8352	-0.0067
39	6	33	38	6	32		88651.462	-0.0155
39	14	26	38	14	25		88656.1169	0.0152
39	14	25	38	14	24		88656.1169	-0.0087
39	13	27	38	13	26		88845.6553	0.1686
39	13	26	38	13	25		88845.6553	-0.2184
38	9	29	37	9	28		88903.8429	0.0029
42	4	39	41	4	38		88937.4541	0.0498
42	3	39	41	3	38		88937.4541	-0.0317
39	12	28	38	12	27		89092.8921	-0.0216
39	12	27	38	12	26		89097.9664	-0.017
43	3	41	42	3	40		89265.228	-0.0016
43	2	41	42	2	40		89265.228	-0.0032
39	8	32	38	8	31		89383.3533	-0.0089
39	11	29	38	11	28		89416.029	0.0128
39	11	28	38	11	27		89467.9288	0.0073
38	7	31	37	7	30		89496.416	-0.0263
44	2	43	43	2	42		89607.2621	-0.0097
44	1	43	43	1	42		89607.2621	-0.0097
39	10	30	38	10	29		89774.8439	-0.0009

39	9	31	38	9	30		89911.1854	0.0445
40	38	2	39	38	1		89936.7361	-0.0678
40	38	3	39	38	2		89936.7361	-0.0678
40	34	6	39	34	5		89981.2833	-0.0236
40	33	7	39	33	6		89994.5472	-0.0722
40	33	8	39	33	7		89994.5472	-0.0722
40	32	9	39	32	8		90009.0693	0.0277
40	32	8	39	32	7		90009.0693	0.0277
40	30	11	39	30	10		90041.8079	-0.039
40	30	10	39	30	9		90041.8079	-0.039
40	28	13	39	28	12		90081.2759	-0.0077
40	28	12	39	28	11		90081.2759	-0.0077
40	7	34	39	7	33		90097.8701	0.0264
40	27	13	39	27	12		90104.1233	-0.0185
40	27	14	39	27	13		90104.1233	-0.0185
40	26	14	39	26	13		90129.5822	0.0356
40	26	15	39	26	14		90129.5822	0.0356
40	25	16	39	25	15		90157.9408	0.0132
40	25	15	39	25	14		90157.9408	0.0132
39	10	29	38	10	28		90162.0821	-0.0097
40	24	17	39	24	16		90189.8139	0.006
40	24	16	39	24	15		90189.8139	0.006
40	23	17	39	23	16		90225.839	0.0071
40	23	18	39	23	17		90225.839	0.0071

40	22	19	39	22	18		90266.7923	-0.0075
40	21	19	39	21	18		90313.7075	-0.0106
40	21	20	39	21	19		90313.7075	-0.0106
40	20	20	39	20	19		90367.8958	0.0283
40	20	21	39	20	20		90367.8958	0.0283
41	5	36	40	5	35		90392.9457	-0.059
40	19	22	39	19	21		90430.886	-0.0164
40	19	21	39	19	20		90430.886	-0.0164
40	6	34	39	6	33		90499.1095	0.0086
40	18	23	39	18	22		90505.0011	0.0039
40	18	22	39	18	21		90505.0011	0.0039
40	17	24	39	17	23		90593.0545	-0.0132
40	17	23	39	17	22		90593.0545	-0.0132
42	5	38	41	5	37		90614.2249	0.0054
42	4	38	41	4	37		90615.7832	-0.0061
40	16	25	39	16	24		90699.13	0.0085
40	16	24	39	16	23		90699.13	0.0084
40	15	25	39	15	24		90828.8645	0.0218
40	15	26	39	15	25		90828.8645	0.0244
43	3	40	42	3	39		90915.7779	-0.0356
43	4	40	42	4	39		90915.7779	0.0123
40	14	26	39	14	25		90990.6184	-0.0232
40	14	27	39	14	26		90990.6184	0.0244
40	13	28	39	13	27		91197.1641	-0.0242

40	13	27	39	13	26	91197.9447	0.0332
44	2	42	43	2	41	91244.9542	0.0119
44	3	42	43	3	41	91244.9542	0.0128
39	7	32	38	7	31	91390.9488	0.0063
40	12	29	39	12	28	91467.4444	0.0034
40	12	28	39	12	27	91476.2987	-0.0049
40	8	33	39	8	32	91510.3759	0.0046
45	2	44	44	2	43	91587.389	-0.0008
45	1	44	44	1	43	91587.389	-0.0008
40	11	30	39	11	29	91814.9242	0.0086
40	11	29	39	11	28	91899.1971	-0.0047
46	0	46	45	0	45	91935.4499	-0.0004
46	1	46	45	1	45	91935.4499	-0.0004
41	7	35	40	7	34	92091.4191	0.0153
40	10	31	39	10	30	92167.9798	0.0133
40	9	32	39	9	31	92206.8947	0.0117
41	36	6	40	36	5	92214.7681	-0.0517
41	36	5	40	36	4	92214.7681	-0.0517
41	35	6	40	35	5	92227.0811	-0.0157
41	35	7	40	35	6	92227.0811	-0.0157
41	34	8	40	34	7	92240.2938	-0.0166
41	34	7	40	34	6	92240.2938	-0.0166
41	33	8	40	33	7	92254.574	-0.0073
41	33	9	40	33	8	92254.574	-0.0073

41	32	9	40	32	8		92270.0733	0.0237
41	32	10	40	32	9		92270.0733	0.0237
41	31	11	40	31	10		92286.8604	-0.0186
41	31	10	40	31	9		92286.8604	-0.0186
41	30	12	40	30	11		92305.23	-0.031
41	30	11	40	30	10		92305.23	-0.031
41	29	12	40	29	11		92325.4167	-0.0046
41	29	13	40	29	12		92325.4167	-0.0046
42	6	37	41	6	36		92331.2509	-0.0115
41	28	14	40	28	13		92347.6278	0.0004
41	28	13	40	28	12		92347.6278	0.0004
41	24	17	40	24	16		92464.3524	-0.0057
41	24	18	40	24	17		92464.3524	-0.0057
41	23	18	40	23	17		92503.083	-0.0583
41	23	19	40	23	18		92503.083	-0.0583
41	22	20	40	22	19		92547.2653	-0.0001
41	22	19	40	22	18		92547.2653	-0.0001
43	5	39	42	5	38		92589.5412	0.0088
43	4	39	42	4	38		92590.4406	-0.0475
41	21	21	40	21	20		92597.8296	0.0089
41	21	20	40	21	19		92597.8296	0.0089
41	20	21	40	20	20		92656.1926	-0.0044
41	20	22	40	20	21		92656.1926	-0.0044
41	19	22	40	19	21		92724.1756	-0.0175

41	19	23	40	19	22		92724.1756	-0.0175
40	10	30	39	10	29		92739.3349	-0.0183
39	8	31	38	8	30		92772.3148	0.0021
41	18	23	40	18	22		92804.1562	-0.0218
41	18	24	40	18	23		92804.1562	-0.0218
44	4	41	43	4	40		92894.28	0.0301
44	3	41	43	3	40		92894.28	0.0022
41	17	25	40	17	24		92899.3569	0.0182
41	17	24	40	17	23		92899.3569	0.0181
41	16	25	40	16	24		93014.0796	0.0053
41	16	26	40	16	25		93014.0796	0.0056
41	15	27	40	15	26		93154.6482	-0.0075
41	15	26	40	15	25		93154.6482	-0.0129
40	7	33	39	7	32		93211.4605	-0.0048
45	3	43	44	3	42		93224.6566	0.0037
45	2	43	44	2	42		93224.6566	0.0032
41	14	28	40	14	27		93330.4271	0.039
41	14	27	40	14	26		93330.4271	-0.0539
41	13	29	40	13	28		93555.6141	0.0947
46	1	45	45	1	44		93567.4679	-0.0026
46	2	45	45	2	44		93567.4679	-0.0026
41	8	34	40	8	33		93605.2953	0.0143
41	12	30	40	12	29		93849.9408	-0.0129
41	12	29	40	12	28		93865.034	-0.1113

47	0	47	46	0	46		93915.5728	-0.0045
47	1	47	46	1	46		93915.5728	-0.0045
42	7	36	41	7	35		94075.208	-0.0007
41	11	31	40	11	30		94219.7118	0.0159
42	6	36	41	6	35		94269.0021	-0.0102
43	6	38	42	6	37		94302.0136	-0.01
43	5	38	42	5	37		94315.4304	-0.0079
41	11	30	40	11	29		94353.7059	-0.0091
40	9	31	39	9	30		94373.9539	0.0056
41	9	33	40	9	32		94471.3167	0.0005
42	35	8	41	35	7		94485.861	-0.019
42	33	9	41	33	8		94515.3003	0.0076
42	32	11	41	32	10		94531.812	-0.0468
42	32	10	41	32	9		94531.812	-0.0468
42	31	11	41	31	10		94549.9343	0.0435
42	31	12	41	31	11		94549.9343	0.0435
41	10	32	40	10	31		94552.1339	-0.0286
44	5	40	43	5	39		94565.3532	0.1486
44	4	40	43	4	39		94565.6875	-0.096
42	30	13	41	30	12		94569.5613	-0.0338
42	29	14	41	29	13		94591.2043	-0.0105
42	29	13	41	29	12		94591.2043	-0.0105
42	28	15	41	28	14		94615.0482	0.0103
42	28	14	41	28	13		94615.0482	0.0103

42	27	16	41	27	15		94641.4258	0.0172
42	27	15	41	27	14		94641.4258	0.0172
42	26	16	41	26	15		94670.7036	-0.0362
42	26	17	41	26	16		94670.7036	-0.0362
42	25	18	41	25	17		94703.5039	-0.0277
42	25	17	41	25	16		94703.5039	-0.0277
42	24	18	41	24	17		94740.3722	-0.0224
42	24	19	41	24	18		94740.3722	-0.0224
42	23	19	41	23	18		94782.1312	0.05
42	23	20	41	23	19		94782.1312	0.05
42	22	21	41	22	20		94829.5417	0.0135
42	22	20	41	22	19		94829.5417	0.0135
45	4	42	44	4	41		94872.8625	0.0235
45	3	42	44	3	41		94872.8625	0.0073
42	21	22	41	21	21		94883.9204	0.0048
42	21	21	41	21	20		94883.9204	0.0048
42	20	23	41	20	22		94946.769	0.0191
42	20	22	41	20	21		94946.769	0.0191
41	7	34	40	7	33		94989.7168	-0.0049
42	19	24	41	19	23		95019.9773	-0.0073
42	19	23	41	19	22		95019.9773	-0.0073
40	8	32	39	8	31		95104.5073	-0.0038
42	18	24	41	18	23		95106.2012	0.0023
42	18	25	41	18	24		95106.2012	0.0023

46	2	44	45	2	43		95204.3459	-0.0133
46	3	44	45	3	43		95204.3459	-0.013
42	17	25	41	17	24		95208.821	-0.0533
42	17	26	41	17	25		95208.821	-0.0533
42	16	26	41	16	25		95332.8263	-0.0123
42	16	27	41	16	26		95332.8263	-0.0117
41	10	31	40	10	30		95370.9677	-0.0285
42	15	27	41	15	26		95485.0002	-0.026
42	15	28	41	15	27		95485.0002	-0.0151
42	8	35	41	8	34		95671.1373	-0.0122
42	14	28	41	14	27		95675.8372	-0.0903
42	14	29	41	14	28		95675.8372	0.0873
48	1	48	47	1	47		95895.6536	-0.0037
48	0	48	47	0	47		95895.6536	-0.0037
42	13	29	41	13	28		95923.2086	0.0052
43	7	37	42	7	36		96052.1042	-0.0088
43	6	37	42	6	36		96183.6322	0.0028
42	12	31	41	12	30		96240.5763	0.0397
42	12	30	41	12	29		96266.089	0.0092
44	6	39	43	6	38		96272.9369	-0.0018
44	5	39	43	5	38		96281.4118	-0.0147
45	5	41	44	5	40		96541.2532	0.0415
45	4	41	44	4	40		96541.2532	-0.3074
42	11	32	41	11	31		96628.5557	0.011

42	9	34	41	9	33	96701.5395	-0.0026
43	36	7	42	36	6	96731.2767	-0.0447
43	36	8	42	36	7	96731.2767	-0.0447
43	35	8	42	35	7	96745.3443	0.0045
43	35	9	42	35	8	96745.3443	0.0045
42	7	35	41	7	34	96756.3262	0.0177
43	34	10	42	34	9	96760.4249	-0.0189
43	34	9	42	34	8	96760.4249	-0.0189
43	33	11	42	33	10	96776.7606	-0.0122
43	33	10	42	33	9	96776.7606	-0.0122
43	32	12	42	32	11	96794.4837	-0.0054
43	32	11	42	32	10	96794.4837	-0.0054
43	30	13	42	30	12	96834.8786	0.0061
43	30	14	42	30	13	96834.8786	0.0061
42	11	31	41	11	30	96837.0779	-0.0409
46	4	43	45	4	42	96851.5277	0.0115
46	3	43	45	3	42	96851.5277	0.002
43	29	15	42	29	14	96858.0198	-0.0031
43	29	14	42	29	13	96858.0198	-0.0031
43	28	15	42	28	14	96883.5435	0.001
43	28	16	42	28	15	96883.5435	0.001
43	27	16	42	27	15	96911.8308	0.0291
43	27	17	42	27	16	96911.8308	0.0291
42	10	33	41	10	32	96922.3143	-0.0319

43	26	17	42	26	16	96943.2827	0.0379
43	26	18	42	26	17	96943.2827	0.0379
43	25	18	42	25	17	96978.4085	-0.0022
43	25	19	42	25	18	96978.4085	-0.0022
43	24	20	42	24	19	97017.9902	0.0328
43	24	19	42	24	18	97017.9902	0.0328
43	23	20	42	23	19	97062.7243	0.0281
43	23	21	42	23	20	97062.7243	0.0281
43	22	21	42	22	20	97113.6349	-0.0038
43	22	22	42	22	21	97113.6349	-0.0038
43	21	22	42	21	21	97172.0717	0.0112
43	21	23	42	21	22	97172.0717	0.0112
47	3	45	46	3	44	97184.0576	0.0032
47	2	45	46	2	44	97184.0576	0.0031
43	20	24	42	20	23	97239.6024	0.0095
43	20	23	42	20	22	97239.6024	0.0095
41	8	33	40	8	32	97309.9227	0.0139
43	19	25	42	19	24	97318.3754	0.0199
43	19	24	42	19	23	97318.3754	0.0199
43	18	25	42	18	24	97411.1269	-0.0277
43	17	26	42	17	25	97521.7866	-0.0054
43	17	27	42	17	26	97521.7866	-0.0053
48	1	47	47	1	46	97527.5188	0.0054
48	2	47	47	2	46	97527.5188	0.0054

43	16	28	42	16	27	97655.5647	-0.0003
43	16	27	42	16	26	97655.5647	-0.0014
43	8	36	42	8	35	97711.7223	0.0014
43	15	29	42	15	28	97820.1547	0.0312
43	15	28	42	15	27	97820.1547	0.0095
44	7	38	43	7	37	98024.4118	0.0056
43	14	29	42	14	28	98027.3417	0.044
43	14	30	42	14	29	98027.3417	0.377
42	10	32	41	10	31	98058.6587	-0.0085
44	6	38	43	6	37	98112.5119	0.0055
45	6	40	44	6	39	98244.2061	-0.0177
43	13	31	42	13	30	98293.4308	-0.0082
43	13	30	42	13	29	98297.6194	-0.0172
46	4	42	45	4	41	98517.6399	-0.0931
43	7	36	42	7	35	98534.4276	0.0362
43	12	31	42	12	30	98681.1969	-0.0072
43	12	31	42	12	30	98681.1969	-0.0072
47	3	44	46	3	43	98830.2581	-0.0142
47	4	44	46	4	43	98830.2581	-0.0088
47	4	44	46	4	43	98830.2581	-0.0088
47	3	44	46	3	43	98830.2581	-0.0142
43	9	35	42	9	34	98895.9417	-0.0056
44	41	3	43	41	2	98929.2639	-0.0149
44	39	5	43	39	4	98951.4404	-0.0298

44	39	6	43	39	5	98951.4404	-0.0298
44	38	6	43	38	5	98963.6	-0.0365
44	38	7	43	38	6	98963.6	-0.0365
44	37	8	43	37	7	98976.6147	-0.0131
44	37	7	43	37	6	98976.6147	-0.0131
44	36	9	43	36	8	98990.5732	0.0309
44	36	8	43	36	7	98990.5732	0.0309
44	35	10	43	35	9	99005.4895	-0.0032
44	35	9	43	35	8	99005.4895	-0.0032
44	34	10	43	34	9	99021.6021	-0.0066
44	34	11	43	34	10	99021.6021	-0.0066
43	11	33	42	11	32	99038.9952	0.0802
44	33	12	43	33	11	99038.9952	-0.0449
44	33	11	43	33	10	99038.9952	-0.0449
44	32	12	43	32	11	99057.9569	-0.0038
44	32	13	43	32	12	99057.9569	-0.0038
44	31	13	43	31	12	99078.5935	0.0199
44	31	14	43	31	13	99078.5935	0.0199
44	30	15	43	30	14	99101.1168	0
44	30	14	43	30	13	99101.1168	0
44	29	15	43	29	14	99125.8902	0.0193
44	29	16	43	29	15	99125.8902	0.0193
44	28	17	43	28	16	99153.1878	0.0191
44	28	16	43	28	15	99153.1878	0.0191

48	3	46	47	3	45	99163.7434	0.0086
48	2	46	47	2	45	99163.7434	0.0086
44	27	18	43	27	17	99183.4187	0.011
44	27	17	43	27	16	99183.4187	0.011
44	26	18	43	26	17	99216.9917	-0.0744
44	26	19	43	26	18	99216.9917	-0.0744
44	25	19	43	25	18	99254.7076	-0.0155
44	25	20	43	25	19	99254.7076	-0.0155
43	10	34	42	10	33	99273.1995	-0.0111
44	24	20	43	24	19	99297.1112	0.0244
44	24	21	43	24	20	99297.1112	0.0244
44	23	21	43	23	20	99345.0869	0.0552
44	23	22	43	23	21	99345.0869	0.0552
43	11	32	42	11	31	99356.4018	0.0314
42	8	34	41	8	33	99387.8758	0.0035
44	22	23	43	22	22	99399.6599	0.0117
44	22	22	43	22	21	99399.6599	0.0117
44	21	24	43	21	23	99462.3039	-0.0104
44	21	23	43	21	22	99462.3039	-0.0104
49	2	48	48	2	47	99507.5001	0.028
49	1	48	48	1	47	99507.5001	0.028
44	20	24	43	20	23	99534.7873	-0.0072
44	20	25	43	20	24	99534.7873	-0.0072
44	19	25	43	19	24	99619.3936	0.0066

44	19	26	43	19	25		99619.3936	0.0066
44	18	26	43	18	25		99719.1565	0.0128
44	18	27	43	18	26		99719.1565	0.0128
44	8	37	43	8	36		99731.0014	-0.0874
42	9	33	41	9	32		99735.8728	0.0223
44	17	28	43	17	27		99838.2399	0.0251
44	17	27	43	17	26		99838.2399	0.025
50	1	50	49	1	49		99855.6735	0.0013
50	0	50	49	0	49		99855.6735	0.0013
44	16	29	43	16	28		99982.4107	-0.0046
44	16	28	43	16	27		99982.4107	-0.007
45	6	39	44	6	38		100052.174	-0.0193
44	15	29	43	15	28		100160.251	0.0089
44	15	30	43	15	29		100160.251	0.0512
46	6	41	45	6	40		100216.009	0.0162
46	5	41	45	5	40		100219.328	0.0078
44	7	37	43	7	36		100337.238	0.0189
47	4	43	46	4	42		100494.164	-0.0704
47	5	43	46	5	42		100494.164	0.0546
44	13	32	43	13	31		100673.694	0.0099
44	13	31	43	13	30		100680.969	0.0164
43	10	33	42	10	32		100795.387	-0.0002
48	4	45	47	4	44		100809.09	0.0119
48	3	45	47	3	44		100809.09	0.0088

44	12	33	43	12	32		101045.114	0.0099
44	9	36	43	9	35		101054.282	-0.0096
44	12	32	43	12	31		101113.33	0.0075
49	3	47	48	3	46		101143.397	0.0009
49	2	47	48	2	46		101143.397	0.0009
45	35	11	44	35	10		101266.365	0.0099
45	35	10	44	35	9		101266.365	0.0099
45	34	12	44	34	11		101283.518	-0.0113
45	34	11	44	34	10		101283.518	-0.0113
45	33	12	44	33	11		101302.073	-0.0402
45	33	13	44	33	12		101302.073	-0.0402
45	32	14	44	32	13		101322.283	-0.0104
45	32	13	44	32	12		101322.283	-0.0104
45	30	16	44	30	15		101368.367	0.0152
45	30	15	44	30	14		101368.367	0.0152
45	29	16	44	29	15		101394.735	-0.0494
45	29	17	44	29	16		101394.735	-0.0494
45	28	18	44	28	17		101423.951	0.0068
45	28	17	44	28	16		101423.951	0.0068
45	27	19	44	27	18		101456.261	0.0039
45	27	18	44	27	17		101456.261	0.0039
45	26	20	44	26	19		101492.243	0.0063
45	26	19	44	26	18		101492.243	0.0063
45	25	21	44	25	20		101532.49	-0.0155

45	25	20	44	25	19		101532.49	-0.0155
45	24	22	44	24	21		101577.835	0.0113
45	24	21	44	24	20		101577.835	0.0113
45	23	22	44	23	21		101629.172	0.0383
45	23	23	44	23	22		101629.172	0.0383
45	22	24	44	22	23		101687.627	0.0177
45	22	23	44	22	22		101687.627	0.0177
45	8	38	44	8	37		101733.414	0.0403
45	21	24	44	21	23		101754.728	-0.0089
45	21	25	44	21	24		101754.728	-0.0089
45	20	26	44	20	25		101832.434	0.0091
45	20	25	44	20	24		101832.434	0.0091
45	19	26	44	19	25		101923.152	-0.0109
45	19	27	44	19	26		101923.152	-0.0109
46	7	40	45	7	39		101961.681	-0.0294
45	17	29	44	17	28		102158.266	-0.0066
45	17	28	44	17	27		102158.266	-0.0069
47	6	42	46	6	41		102188.301	0.0112
47	5	42	46	5	41		102190.346	-0.0085
43	9	34	42	9	33		102292.525	-0.0044
45	16	29	44	16	28		102313.556	-0.0089
45	16	30	44	16	29		102313.556	-0.004
48	4	44	47	4	43		102470.987	-0.0242
48	5	44	47	5	43		102470.987	0.0502

45	15	30	44	15	29		102505.507	-0.0523
45	15	31	44	15	30		102505.507	0.0287
45	14	32	44	14	31		102748.233	0.045
45	14	31	44	14	30		102749.293	-0.0031
49	3	46	48	3	45		102787.943	0.004
49	4	46	48	4	45		102787.943	0.0058
45	13	33	44	13	32		103061.81	-0.0117
50	3	48	49	3	47		103123.034	-0.0006
50	2	48	49	2	47		103123.034	-0.0006
45	9	37	44	9	36		103177.608	-0.0672
44	8	36	43	8	35		103205.053	-0.0235
46	40	6	45	40	5		103453.888	-0.0263
45	12	34	44	12	33		103457.785	-0.0184
46	37	10	45	37	9		103495.191	-0.0582
46	36	11	45	36	10		103510.943	-0.0588
46	36	10	45	36	9		103510.943	-0.0588
46	35	12	45	35	11		103527.879	-0.0645
46	35	11	45	35	10		103527.879	-0.0645
46	34	13	45	34	12		103546.216	-0.0068
46	34	12	45	34	11		103546.216	-0.0068
44	10	34	43	10	33		103562.456	-0.0146
45	12	33	44	12	32		103566	-0.1636
46	33	14	45	33	13		103566	-0.0118
46	32	15	45	32	14		103587.493	-0.0161

46	32	14	45	32	13		103587.493	-0.0161
46	31	15	45	31	14		103610.953	0.0061
46	31	16	45	31	15		103610.953	0.0061
46	30	16	45	30	15		103636.615	0.0156
46	30	17	45	30	16		103636.615	0.0156
46	29	17	45	29	16		103664.797	0.0081
46	29	18	45	29	17		103664.797	0.0081
46	28	18	45	28	17		103695.892	-0.0052
46	28	19	45	28	18		103695.892	-0.0052
46	27	20	45	27	19		103730.415	0.0339
46	27	19	45	27	18		103730.415	0.0339
46	26	21	45	26	20		103768.82	0.0293
46	26	20	45	26	19		103768.82	0.0293
46	25	21	45	25	20		103811.777	-0.0183
46	25	22	45	25	21		103811.777	-0.0183
52	0	52	51	0	51		103815.476	-0.0112
52	1	52	51	1	51		103815.476	-0.0112
45	11	35	44	11	34		103850.093	-0.0124
45	10	36	44	10	35		103896.856	0.0624
46	23	24	45	23	23		103915.046	-0.0035
46	23	23	45	23	22		103915.046	-0.0035
47	7	41	46	7	40		103928.882	-0.0288
47	6	41	46	6	40		103953.745	-0.0247
46	22	25	45	22	24		103977.594	0.0184

46	22	24	45	22	23		103977.594	0.0184
46	7	39	45	7	38		104029.889	-0.019
46	21	25	45	21	24		104049.4	0.0087
46	21	26	45	21	25		104049.4	0.0087
46	20	27	45	20	26		104132.568	0.0112
46	20	26	45	20	25		104132.568	0.0112
48	6	43	47	6	42		104161.135	0.0151
48	5	43	47	5	42		104162.407	0.0132
46	19	28	45	19	27		104229.767	-0.0028
46	19	27	45	19	26		104229.767	-0.0028
46	18	28	45	18	27		104344.637	0.0011
46	18	29	45	18	28		104344.637	0.0011
49	5	45	48	5	44		104448.003	0.0258
49	4	45	48	4	44		104448.003	-0.0183
46	17	30	45	17	29		104482.103	0.002
46	17	29	45	17	28		104482.103	0.0015
45	11	34	44	11	33		104533.947	0.0097
46	16	31	45	16	30		104649.208	0.0279
46	16	30	45	16	29		104649.208	0.0181
44	9	35	43	9	34		104734.277	-0.0319
50	4	47	49	4	46		104766.827	-0.0073
50	3	47	49	3	46		104766.827	-0.0083
46	15	31	45	15	30		104856.304	-0.0629
46	15	32	45	15	31		104856.304	0.0894

45	8	37	44	8	36		104991.984	0.0272
51	3	49	50	3	48		105102.669	0.0221
51	2	49	50	2	48		105102.669	0.0221
46	14	33	45	14	32		105118.874	0.0207
46	9	38	45	9	37		105268.422	0.0261
52	1	51	51	1	50		105447.104	0.0242
52	2	51	51	2	50		105447.104	0.0242
46	13	33	45	13	32		105478.704	0.0216
47	8	40	46	8	39		105701.763	0.0074
47	38	10	46	38	9		105739.895	-0.045
47	37	10	46	37	9		105755.5	-0.0394
47	37	11	46	37	10		105755.5	-0.0394
47	36	12	46	36	11		105772.255	-0.0167
47	36	11	46	36	10		105772.255	-0.0167
47	35	12	46	35	11		105790.241	-0.0342
47	35	13	46	35	12		105790.241	-0.0342
53	1	53	52	1	52		105795.29	-0.0265
53	0	53	52	0	52		105795.29	-0.0265
47	33	14	46	33	13		105830.792	0.0383
47	33	15	46	33	14		105830.792	0.0383
47	32	15	46	32	14		105853.614	-0.0122
47	32	16	46	32	15		105853.614	-0.0122
47	31	17	46	31	16		105878.614	0.0411
47	31	16	46	31	15		105878.614	0.0411

48	7	42	47	7	41		105896.07	0.0187
47	30	18	46	30	17		105905.872	-0.0142
47	30	17	46	30	16		105905.872	-0.0142
48	6	42	47	6	41		105912.099	0.0281
47	7	40	46	7	39		105914.933	-0.0106
47	29	19	46	29	18		105935.927	0.0163
47	29	18	46	29	17		105935.927	0.0163
47	28	19	46	28	18		105969.079	0.0234
47	28	20	46	28	19		105969.079	0.0234
47	27	20	46	27	19		106005.834	0.0247
47	27	21	46	27	20		106005.834	0.0247
46	12	34	45	12	33		106044.588	-0.0099
47	26	21	46	26	20		106046.77	0.008
47	26	22	46	26	21		106046.77	0.008
47	25	23	46	25	22		106092.633	0.0027
47	25	22	46	25	21		106092.633	0.0027
49	6	44	48	6	43		106134.489	0.0259
49	5	44	48	5	43		106135.201	-0.0435
47	24	23	46	24	22		106144.313	0.024
47	24	24	46	24	23		106144.313	0.024
46	10	37	45	10	36		106161.069	0.0361
47	23	24	46	23	23		106202.851	0.0248
47	23	25	46	23	24		106202.851	0.0248
47	22	26	46	22	25		106269.631	0.0303

47	22	25	46	22	24		106269.631	0.0303
45	10	35	44	10	34		106329.728	-0.0074
47	21	27	46	21	26		106346.384	0.0451
47	21	26	46	21	25		106346.384	0.0451
50	4	46	49	4	45		106425.225	-0.0052
50	5	46	49	5	45		106425.225	0.0208
47	20	27	46	20	26		106435.277	0.0122
47	20	28	46	20	27		106435.277	0.0122
47	19	29	46	19	28		106539.304	0.0055
47	19	28	46	19	27		106539.304	0.0055
47	18	29	46	18	28		106662.372	0.0137
47	18	30	46	18	29		106662.372	0.0138
46	8	38	45	8	37		106740.83	-0.0021
51	3	48	50	3	47		106745.765	0.0041
51	4	48	50	4	47		106745.765	0.0047
47	17	30	46	17	29		106809.812	-0.0355
47	17	31	46	17	30		106809.812	-0.0344
47	16	32	46	16	31		106989.468	-0.0026
47	16	31	46	16	30		106989.468	-0.0218
45	9	36	44	9	35		107047.444	-0.0204
52	2	50	51	2	49		107082.226	-0.0039
52	3	50	51	3	49		107082.226	-0.0039
46	11	35	45	11	34		107205.535	0.0073
47	15	33	46	15	32		107212.789	0.1103

47	15	32	46	15	31		107212.789	-0.1713
47	9	39	46	9	38		107329.699	-0.0032
53	2	52	52	2	51		107426.874	0.0201
53	1	52	52	1	51		107426.874	0.0201
47	14	33	46	14	32		107500.098	-0.0107
48	8	41	47	8	40		107674.162	-0.0285
54	1	54	53	1	53		107775.086	-0.0068
54	0	54	53	0	53		107775.086	-0.0068
47	13	35	46	13	34		107862.295	0.0213
49	7	43	48	7	42		107863.513	-0.001
49	6	43	48	6	42		107873.757	-0.0024
47	13	34	46	13	33		107896.23	0.0049
48	39	9	47	39	8		107984.489	-0.0058
48	37	12	47	37	11		108016.453	-0.0488
48	36	12	47	36	11		108034.217	-0.0385
48	34	15	47	34	14		108074.006	0.0047
48	34	14	47	34	13		108074.006	0.0047
48	33	16	47	33	15		108096.363	0.0037
48	33	15	47	33	14		108096.363	0.0037
50	6	45	49	6	44		108108.387	0.1045
50	5	45	49	5	44		108108.66	-0.0994
48	31	17	47	31	16		108147.199	0.012
48	31	18	47	31	17		108147.199	0.012
48	30	18	47	30	17		108176.298	0.0639

48	30	19	47	30	18		108176.298	0.0639
48	29	20	47	29	19		108208.196	0.0212
48	29	19	47	29	18		108208.196	0.0212
48	28	20	47	28	19		108243.42	-0.0277
48	28	21	47	28	20		108243.42	-0.0277
48	27	21	47	27	20		108282.604	0.0304
48	27	22	47	27	21		108282.604	0.0304
47	12	36	46	12	35		108296.938	-0.0128
48	26	23	47	26	22		108326.187	0.0019
48	26	22	47	26	21		108326.187	0.0019
48	25	23	47	25	22		108375.054	0.0054
48	25	24	47	25	23		108375.054	0.0054
47	10	38	46	10	37		108389.604	-0.0168
51	4	47	50	4	46		108402.594	-0.0155
51	5	47	50	5	46		108402.594	-0.0002
48	24	24	47	24	23		108430.082	-0.0207
48	24	25	47	24	24		108430.082	-0.0207
47	8	39	46	8	38		108482.734	-0.0103
48	23	26	47	23	25		108492.533	0.0205
48	23	25	47	23	24		108492.533	0.0205
47	12	35	46	12	34		108554.818	0.0232
48	22	27	47	22	26		108563.747	0.0054
48	22	26	47	22	25		108563.747	0.0054
47	11	37	46	11	36		108618.131	0.01

48	21	28	47	21	27		108645.643	-0.0028
48	21	27	47	21	26		108645.643	-0.0028
52	3	49	51	3	48		108724.679	-0.0268
52	4	49	51	4	48		108724.679	-0.0265
48	20	28	47	20	27		108740.649	0.023
48	20	29	47	20	28		108740.649	0.023
48	19	30	47	19	29		108851.861	0.0181
48	19	29	47	19	28		108851.861	0.0181
48	18	31	47	18	30		108983.545	-0.008
48	18	30	47	18	29		108983.545	-0.0081
46	10	36	45	10	35		109060.152	-0.0205
53	3	51	52	3	50		109061.776	-0.0038
53	2	51	52	2	50		109061.776	-0.0038
48	17	31	47	17	30		109141.653	-0.008
48	17	32	47	17	31		109141.653	-0.0057
46	9	37	45	9	36		109225.603	-0.0532
48	16	33	47	16	32		109334.659	0.0175
48	16	32	47	16	31		109334.659	-0.0192
48	9	40	47	9	39		109365.46	-0.0288
54	2	53	53	2	52		109406.609	0.0303

S3.3 Linelist for CHT-1-CN-2 in vibrational ground state

Measured frequencies and residuals (in MHz) for the rotational transitions of CHT-1-CN-1 in 2-26 GHz using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	F	J'	K'_a	K'_c	F'	Observed	Residuals
								Freq. (MHz)	(MHz)
5	3	3	6	5	2	3	6	2535.9323	0.0153
5	3	3	5	5	2	3	5	2536.4583	0.0125
4	3	2	3	4	2	2	3	2750.3573	0.0224
4	3	2	5	4	2	2	5	2750.4636	0.0204
4	3	2	4	4	2	2	4	2750.874	0.0095
3	3	1	3	3	2	1	4	2880.2676	0.0095
3	3	1	2	3	2	1	2	2880.2676	0.0049
3	3	1	4	3	2	1	4	2880.3624	0.0054
3	3	1	4	3	2	1	4	2880.3624	0.0054
3	3	1	3	3	2	1	3	2880.617	-0.0088
3	3	1	3	3	2	1	3	2880.617	-0.0088
1	1	0	1	0	0	0	1	3934.3653	-0.0025
1	1	0	2	0	0	0	1	3935.0474	-0.0038
2	1	2	1	1	1	1	1	6422.7084	0.0197
2	1	2	3	1	1	1	2	6423.7544	0.015
2	1	2	2	1	1	1	1	6423.7544	-0.0732
2	1	2	1	1	1	1	0	6424.3086	0.0099

2	1	2	2	1	1	1	2	6424.4843	0.0127
2	0	2	1	1	0	1	1	6531.8899	0.0024
2	0	2	3	1	0	1	2	6532.0343	0
2	0	2	1	1	0	1	0	6532.196	0.2102
2	0	2	2	1	0	1	1	6532.196	0.0077
2	1	1	1	1	1	0	0	6681.498	-0.0306
2	1	1	2	1	1	0	2	6681.498	0.0177
2	1	1	2	1	1	0	1	6682.164	0.0003
2	1	1	3	1	1	0	2	6682.164	-0.0064
2	1	1	1	1	1	0	1	6683.2225	-0.0147
2	1	1	2	1	0	1	1	7340.0097	-0.0026
2	1	1	2	1	0	1	2	7340.0097	-0.0419
2	1	1	3	1	0	1	2	7340.7255	-0.0161
2	1	1	1	1	0	1	1	7341.0543	-0.0314
2	1	1	1	1	0	1	0	7341.1474	-0.0366
2	1	1	1	1	0	1	0	7341.1668	-0.0173
2	2	0	1	1	1	0	0	8289.895	0.0152
2	2	0	2	1	1	0	2	8290.6048	0.0009
2	2	0	3	1	1	0	2	8290.8041	0.0069
2	2	0	2	1	1	0	1	8291.2876	0.0003
2	2	0	1	1	1	0	1	8291.5883	-0.0001
2	2	1	2	1	1	1	1	8398.5642	-0.0153
2	2	1	3	1	1	1	2	8399.2383	-0.0274
5	1	4	5	4	0	4	4	18050.0279	-0.0214

5	1	4	6	4	0	4	5	18051.0793	-0.0369
5	1	4	4	4	0	4	3	18051.3617	-0.0063
5	2	3	4	4	1	3	3	18114.9144	0.0424
5	2	3	6	4	1	3	5	18114.9144	0.0334
5	2	3	5	4	1	3	4	18114.9144	0.136
5	2	4	5	4	1	4	4	18794.6862	-0.0205
6	1	6	7	5	1	5	6	19152.8237	-0.0303
6	1	6	6	5	1	5	5	19152.8237	-0.1048
6	1	6	5	5	1	5	4	19152.8237	-0.0517
6	0	6	6	5	0	5	5	19202.0918	-0.16
6	0	6	7	5	0	5	6	19202.0918	-0.0152
6	0	6	5	5	0	5	4	19202.0918	-0.02
5	3	2	6	4	2	2	5	19242.2858	0.0577
5	3	2	5	4	2	2	4	19242.5437	0.0392
5	3	3	4	4	2	3	5	19468.4489	-0.035
5	3	3	6	4	2	3	5	19468.4489	-0.0076
6	2	5	6	5	2	4	5	19566.1049	-0.0966
6	2	5	5	5	2	4	4	19566.1049	-0.0068
6	2	5	7	5	2	4	6	19566.1049	-0.016
6	3	4	6	5	3	3	5	19723.756	0.0082
6	3	4	7	5	3	3	6	19723.756	0.0072
6	3	4	5	5	3	3	4	19723.756	0.0117
6	4	3	5	5	4	2	4	19727.7319	0.036
6	4	3	6	5	4	2	5	19727.7319	0.0642

6	4	3	7	5	4	2	6	19727.7319	0.0364
6	4	2	6	5	4	1	5	19734.0422	0.0342
6	4	2	7	5	4	1	6	19734.0422	-0.0064
6	4	2	5	5	4	1	4	19734.0422	-0.0087
6	1	5	6	5	1	4	5	19822.5106	-0.0803
6	1	5	7	5	1	4	6	19822.5106	0.1037
6	1	5	5	5	1	4	4	19822.5106	0.1495
6	3	3	5	5	3	2	4	19829.1122	0.0175
6	3	3	6	5	3	2	5	19829.1122	0.1567
6	3	3	7	5	3	2	6	19829.1122	0.0297
6	2	4	5	5	2	3	4	20016.0724	0.0353
6	2	4	6	5	2	3	5	20016.0724	0.0717
6	2	4	7	5	2	3	6	20016.0724	0.0207
5	4	1	4	4	3	1	5	20540.6235	-0.0031
5	4	1	6	4	3	1	5	20540.6235	0.0235
5	4	1	4	4	3	1	3	20540.6235	0.041
5	4	2	4	4	3	2	3	20553.7784	0.0108
5	4	2	5	4	3	2	4	20553.7784	0.01
5	4	2	6	4	3	2	5	20553.7784	0.0053
6	2	4	6	5	1	4	5	21540.1652	0.0154
6	2	4	7	5	1	4	6	21540.4797	0.0395
6	2	4	5	5	1	4	4	21540.4797	0.0053
5	5	0	5	4	4	0	4	21730.4295	0.0864
5	5	1	4	4	4	1	3	21730.4295	-0.0744

5	5	1	6	4	4	1	5	21730.4295	-0.08
5	5	0	4	4	4	0	3	21730.4295	0.0942
5	5	0	6	4	4	0	5	21730.4295	0.0884
5	5	1	5	4	4	1	4	21730.4295	-0.0812
6	1	5	6	5	0	5	5	21804.8257	-0.0237
6	1	5	5	5	0	5	4	21806.0348	-0.1048
6	1	5	7	5	0	5	6	21806.0348	0.1066
6	3	3	7	5	2	3	6	22422.2774	-0.0877
6	3	3	5	5	2	3	4	22422.2774	-0.0188
6	3	3	7	5	2	3	6	22422.2784	-0.0867
6	3	3	5	5	2	3	4	22422.2784	-0.0178
6	3	3	6	5	2	3	5	22422.6536	0.0174
6	3	3	6	5	2	3	5	22422.6536	0.0174
6	3	4	6	5	2	4	5	22856.0284	-0.0647
6	3	4	7	5	2	4	6	22856.3461	-0.0076
7	4	3	8	6	4	2	7	23051.6518	-0.0358
7	4	3	6	6	4	2	5	23051.6518	-0.0398
7	4	3	7	6	4	2	6	23051.6518	0.021
7	3	4	8	6	3	3	7	23213.499	-0.03
7	3	4	6	6	3	3	5	23213.499	-0.0408
7	3	4	7	6	3	3	6	23213.499	0.1121
7	2	5	6	6	2	4	5	23355.2002	0.0479
7	2	5	7	6	2	4	6	23355.2002	0.0125
7	2	5	8	6	2	4	7	23355.2002	0.028

6	4	3	5	5	3	3	4	23847.0088	-0.0389
6	4	3	6	5	3	3	5	23847.0088	-0.0224
6	4	3	7	5	3	3	6	23847.0088	-0.0406
6	5	1	6	5	4	1	5	25011.9503	-0.0185
6	5	1	5	5	4	1	4	25011.9503	-0.0012
6	5	1	7	5	4	1	6	25011.9503	-0.0076
6	5	2	5	5	4	2	4	25013.427	0.0029
6	5	2	7	5	4	2	6	25013.427	-0.0026
6	5	2	6	5	4	2	5	25013.427	-0.0088

S4.0 The experimental rotational constants for the heavy-atom isotopologues

Experimental rotational constants obtained for the observed isotopologues of CHT-1-CN-1. Parameters are obtained by using the SPFIT program for the 2-26 GHz region.

Rotational parameters	¹³ C1	¹³ C2	¹³ C3	¹³ C4	¹³ C8	¹⁵ N7
A ^a /MHz	3536.684(45)	3497.122(23)	3480.336(25)	3523.275(27)	3536.827(64)	3537.177(34)
B (MHz)	1249.65504(70)	1250.77571(70)	1247.06586(48)	1237.20758(55)	1236.6123(12)	1217.87199(73)
C (MHz)	989.65546(53)	987.70952(45)	983.63065(36)	981.12660(47)	981.4223(12)	969.55357(64)
Δ_J^b /kHz	[0.055512]	[0.055512]	[0.055512]	[0.055512]	[0.055512]	[0.055512]
Δ_{JK} /kHz	[0.20096]	[0.20096]	[0.20096]	[0.20096]	[0.20096]	[0.20096]
Δ_K /kHz	[0.83]	[0.83]	[0.83]	[0.83]	[0.83]	[0.83]
δ_J /kHz	[-0.0067]	[-0.0067]	[-0.0067]	[-0.0067]	[-0.0067]	[-0.0067]
δ_K /kHz	[-0.27771]	[-0.27771]	[-0.27771]	[-0.27771]	[-0.27771]	[-0.27771]
χ_{aa}^c /MHz	-4.245(14)	-4.242(14)	-4.241(10)	-4.241(13)	-4.234(22)	-
χ_{bb-cc} /MHz	[0.00772]	[0.00772]	[0.00772]	[0.00772]	[0.00772]	-

^a A, B, and C are the rotational constants

^b Δ_J , Δ_{JK} , Δ_K , δ_J , and δ_K are the quartic centrifugal distortion constants.

^c χ_{aa} , χ_{bb} , and χ_{cc} represent the diagonal elements of the ¹⁴N nuclear quadrupole coupling tensor.

S5.0 List of rotational transitions for singly-substituted heavy-atom isotopologues of CHT-1-CN-1

S5.1 Measured frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}1$ CHT-1-CN-1 in the low-frequency region (2-26 GHz) fit using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	F	J'	K'_a	K'_c	F'	Observed Freq. (MHz)	Residuals (MHz)
2	1	2	2	1	1	1	1	4217.569	0.0094
2	1	2	2	1	1	1	2	4218.2176	0.0101
2	1	2	1	1	1	1	1	4218.6048	0.0028
2	1	2	3	1	1	1	2	4218.8818	0.0047
2	1	2	1	1	1	1	0	4220.2262	0.0041
2	0	2	2	1	0	1	2	4456.4201	-0.0012
2	0	2	1	1	0	1	0	4456.6241	0.0018
2	0	2	2	1	0	1	1	4457.7011	0.0067
2	0	2	3	1	0	1	2	4457.7789	0.0008
3	1	3	3	2	1	2	3	6314.4095	0.0088
3	1	3	3	2	1	2	2	6315.0769	0.0065
3	1	3	4	2	1	2	3	6315.4516	0.0048
3	1	3	2	2	1	2	1	6315.4516	0.0112
3	1	3	2	2	1	2	2	6316.4871	0.0043
3	0	3	3	2	0	2	3	6633.7413	-0.0007

3	0	3	2	2	0	2	1	6634.8759	0.0027
3	0	3	3	2	0	2	2	6635.1298	0.0308
3	0	3	4	2	0	2	3	6635.1298	-0.0087
3	2	2	2	2	2	1	2	6716.8704	0.0102
3	2	2	3	2	2	1	2	6716.8704	0.0105
3	2	2	4	2	2	1	3	6718.2374	0.0135
3	2	1	3	2	2	0	2	6799.6775	-0.0088
3	2	1	4	2	2	0	3	6801.0652	0.0038
3	2	1	2	2	2	0	1	6801.8184	-0.0037
3	1	2	3	2	1	1	3	7093.3044	-0.0085
3	1	2	3	2	1	1	2	7093.9992	-0.0083
3	1	2	2	2	1	1	1	7094.3753	0.0021
3	1	2	4	2	1	1	3	7094.3753	-0.009
4	1	4	4	3	1	3	3	8398.2591	0.0018
4	1	4	5	3	1	3	4	8398.4208	-0.0019
4	1	4	3	3	1	3	2	8398.4208	0.0528
4	0	4	3	3	0	3	2	8755.5259	0.0037
4	0	4	4	3	0	3	3	8755.6445	0.0158
4	0	4	5	3	0	3	4	8755.6445	-0.0028
4	1	3	4	3	1	2	3	9431.9215	-0.0109
4	1	3	3	3	1	2	2	9432.0215	-0.0185
4	1	3	5	3	1	2	4	9432.0954	-0.0018
8	1	7	8	7	1	6	7	18408.8893	0.0061
8	1	7	9	7	1	6	8	18408.8893	-0.0082

8	1	7	7	7	1	6	6		18408.8893	0.0156
9	1	9	9	8	1	8	8		18577.3425	0.0299
9	1	9	10	8	1	8	9		18577.3425	0.0127
9	1	9	8	8	1	8	7		18577.3425	0.0308
9	0	9	8	8	0	8	7		18694.1156	0.0459
9	0	9	9	8	0	8	8		18694.1156	0.0323
9	0	9	10	8	0	8	9		18694.1156	0.0262
8	2	6	8	7	2	5	7		18823.3409	0.055
8	2	6	7	7	2	5	6		18823.3409	-0.0106
8	2	6	9	7	2	5	8		18823.3409	0.055
10	1	10	9	9	1	9	8		20576.0341	-0.0315
10	1	10	11	9	1	9	10		20576.0341	-0.0463
10	1	10	10	9	1	9	9		20576.0341	-0.0333
10	0	10	11	9	0	9	10		20652.1322	-0.0312
10	0	10	10	9	0	9	9		20652.1322	-0.0245
10	0	10	9	9	0	9	8		20652.1322	-0.0155
11	1	11	11	10	1	10	10		22568.0764	-0.0094
11	1	11	12	10	1	10	11		22568.0764	-0.0197
11	1	11	10	10	1	10	9		22568.0764	-0.0073

S5.2 Measured frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}2$ CHT-1-CN-1 in the low-frequency region (2-26 GHz) fit using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	F	J'	K'_a	K'_c	F'	Observed Freq. (MHz)	Residuals (MHz)
2	1	2	2	1	1	1	2	4213.4936	0.0029
2	1	2	1	1	1	1	1	4213.8868	0.0019
2	1	2	3	1	1	1	2	4214.1633	0.0034
2	0	2	2	1	0	1	2	4453.926	0.001
2	0	2	1	1	0	1	0	4454.1273	0.0019
2	0	2	2	1	0	1	1	4455.2056	0.0081
2	0	2	3	1	0	1	2	4455.2841	0.0032
2	0	2	1	1	0	1	1	4457.3099	0.0027
2	1	1	2	1	1	0	1	4738.9744	0.0016
2	1	1	3	1	1	0	2	4740.2914	0.0001
3	1	3	3	2	1	2	3	6306.8342	0.0047
3	1	3	3	2	1	2	2	6307.503	0.0043
3	1	3	2	2	1	2	1	6307.8779	0.0094
3	1	3	4	2	1	2	3	6307.8779	0.0031
3	1	3	2	2	1	2	2	6308.9144	0.004
3	0	3	3	2	0	2	3	6627.9741	0.0053
3	0	3	2	2	0	2	1	6629.1027	0.0044
3	0	3	3	2	0	2	2	6629.357	0.0324

3	0	3	4	2	0	2	3	6629.357	-0.0065
3	0	3	2	2	0	2	2	6631.2104	0.0024
3	2	2	3	2	2	1	2	6714.3888	0.0042
3	2	2	4	2	2	1	3	6715.7507	0.0027
3	2	2	2	2	2	1	1	6716.5073	0.0015
3	2	1	3	2	2	0	2	6800.5043	-0.0054
3	2	1	4	2	2	0	3	6801.8848	0.0001
3	2	1	2	2	2	0	1	6802.6429	-0.0021
3	1	2	3	2	1	1	3	7094.8664	-0.0008
3	1	2	3	2	1	1	2	7095.5592	-0.0021
3	1	2	4	2	1	1	3	7095.9329	-0.005
3	1	2	2	2	1	1	1	7095.9329	0.0062
4	1	4	4	3	1	3	3	8387.3316	-0.0021
4	1	4	5	3	1	3	4	8387.4965	-0.0025
8	1	7	9	7	1	6	8	18389.6765	0.0149
8	1	7	7	7	1	6	6	18389.6765	0.0387
8	1	7	8	7	1	6	7	18389.6765	0.0284
9	1	9	9	8	1	8	8	18544.0466	0.0298
9	1	9	8	8	1	8	7	18544.0466	0.0307
9	1	9	10	8	1	8	9	18544.0466	0.0127
9	0	9	9	8	0	8	8	18654.6374	0.0377
9	0	9	8	8	0	8	7	18654.6374	0.0509
9	0	9	10	8	0	8	9	18654.6374	0.0313
8	2	6	8	7	2	5	7	18834.6203	0.0854

8	2	6	9	7	2	5	8	18834.6203	0.0077
8	2	6	7	7	2	5	6	18834.6203	0.0205
9	2	8	9	8	2	7	8	19768.4814	0.0005
9	2	8	10	8	2	7	9	19768.4814	-0.0511
9	2	8	8	8	2	7	7	19768.4814	-0.0393
9	1	8	9	8	1	7	8	20475.0612	-0.0226
9	1	8	8	8	1	7	7	20475.0612	-0.0082
9	1	8	10	8	1	7	9	20475.0612	-0.0276
10	1	10	11	9	1	9	10	20538.052	-0.0345
10	1	10	10	9	1	9	9	20538.052	-0.0215
10	1	10	9	9	1	9	8	20538.052	-0.0197
10	0	10	10	9	0	9	9	20609.3114	-0.0153
10	0	10	9	9	0	9	8	20609.3114	-0.0066
10	0	10	11	9	0	9	10	20609.3114	-0.0222
10	2	9	9	9	2	8	8	21864.7435	0.0229
10	2	9	11	9	2	8	10	21864.7435	0.012
10	2	9	10	9	2	8	9	21864.7435	0.0489
10	1	9	9	9	1	8	8	22492.0307	0.0095
10	1	9	11	9	1	8	10	22492.0307	-0.0064
10	1	9	10	9	1	8	9	22492.0307	-0.0061
11	1	11	10	10	1	10	9	22525.5209	-0.0131
11	1	11	12	10	1	10	11	22525.5209	-0.0254
11	1	11	11	10	1	10	10	22525.5209	-0.0151
10	2	8	11	9	2	7	10	23562.6355	-0.0598

10	2	8	10	9	2	7	9	23562.6355	-0.0267
10	2	8	9	9	2	7	8	23562.6355	-0.0477
11	1	10	12	10	1	9	11	24455.3063	0.0095
11	1	10	11	10	1	9	10	24455.3063	0.0082
12	0	12	11	11	0	11	10	24535.4801	0
12	0	12	12	11	0	11	11	24535.4801	-0.004
12	0	12	13	11	0	11	12	24535.4801	-0.0105

S5.3 Measured frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}3$ CHT-1-CN-1 in the low-frequency region (2-26 GHz) fit using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	F	J'	K'_a	K'_c	F'	Observed Freq. (MHz)	Residuals (MHz)
2	1	2	2	1	1	1	1	4196.9008	0.00395
2	1	2	2	1	1	1	2	4197.5505	0.00616
2	1	2	1	1	1	1	1	4197.9411	0.00274
2	1	2	3	1	1	1	2	4198.2196	0.00636
2	1	2	1	1	1	1	0	4199.5631	0.00595
2	0	2	2	1	0	1	2	4438.1664	-0.00209
2	0	2	2	1	0	1	1	4439.4441	0.0035
2	0	2	3	1	0	1	2	4439.5268	0.00298
2	0	2	1	1	0	1	1	4441.5539	0.00459
2	1	1	2	1	1	0	1	4723.7662	0.00148
2	1	1	2	1	1	0	2	4724.3964	0.00752
2	1	1	1	1	1	0	1	4724.8483	0.00352
2	1	1	3	1	1	0	2	4725.0857	0.00302
2	1	1	1	1	1	0	0	4726.4002	-0.00526
3	1	3	3	2	1	2	3	6282.8169	0.01137
3	1	3	3	2	1	2	2	6283.4875	0.01299
3	1	3	2	2	1	2	1	6283.8599	0.0159
3	1	3	4	2	1	2	3	6283.8599	0.00954

3	1	3	2	2	1	2	2	6284.8929	0.00736
3	0	3	3	2	0	2	3	6603.9084	0.00193
3	0	3	2	2	0	2	1	6605.0382	0.00285
3	0	3	3	2	0	2	2	6605.2917	0.02993
3	0	3	4	2	0	2	3	6605.2917	-0.00888
3	0	3	2	2	0	2	2	6607.1417	-0.00246
3	2	2	2	2	2	1	2	6691.0222	0.00307
3	2	2	3	2	2	1	2	6691.0222	0.00338
3	2	2	3	2	2	1	3	6692.3853	0.00352
3	2	2	4	2	2	1	3	6692.3853	0.00367
3	2	2	2	2	2	1	1	6693.1453	0.00609
3	2	1	3	2	2	0	2	6777.8376	-0.00288
3	2	1	4	2	2	0	3	6779.2161	0.00101
3	2	1	2	2	2	0	1	6779.9742	-0.00104
3	1	2	3	2	1	1	3	7071.9252	-0.00807
3	1	2	3	2	1	1	2	7072.6177	-0.00937
3	1	2	2	2	1	1	1	7072.9956	0.00327
3	1	2	4	2	1	1	3	7072.9956	-0.00794
3	1	2	2	2	1	1	2	7074.0677	-0.0046
4	1	4	4	3	1	3	3	8355.1343	0.00526
4	1	4	3	3	1	3	2	8355.2914	0.05201
4	1	4	5	3	1	3	4	8355.2914	-0.00272
4	0	4	3	3	0	3	2	8711.7213	-0.00343
4	0	4	4	3	0	3	3	8711.8487	0.01677

4	0	4	5	3	0	3	4	8711.8487	-0.00107
4	2	2	4	3	2	1	3	9116.1303	0.00309
4	2	2	5	3	2	1	4	9116.7214	0.00354
4	2	2	3	3	2	1	2	9116.8582	-0.00963
8	1	7	8	7	1	6	7	18323.4241	0.00461
8	1	7	7	7	1	6	6	18323.4241	0.01511
8	1	7	9	7	1	6	8	18323.4241	-0.0087
9	1	9	8	8	1	8	7	18469.9323	0.04328
9	1	9	10	8	1	8	9	18469.9323	0.02522
9	1	9	9	8	1	8	8	18469.9323	0.04236
9	0	9	9	8	0	8	8	18578.8501	0.01779
9	0	9	10	8	0	8	9	18578.8501	0.01135
9	0	9	8	8	0	8	7	18578.8501	0.03094
8	2	6	9	7	2	5	8	18775.2582	-0.00954
8	2	6	7	7	2	5	6	18775.2582	0.00324
8	2	6	8	7	2	5	7	18775.2582	0.06798
9	2	8	8	8	2	7	7	19695.4902	-0.00404
9	2	8	10	8	2	7	9	19695.4902	-0.01581
9	2	8	9	8	2	7	8	19695.4902	0.03577
9	1	8	8	8	1	7	7	20398.8166	0.02071
9	1	8	9	8	1	7	8	20398.8166	0.0061
9	1	8	10	8	1	7	9	20398.8166	0.00128
10	1	10	9	9	1	9	8	20455.5426	-0.0223
10	1	10	11	9	1	9	10	20455.5426	-0.03711

10	1	10	10	9	1	9	9	20455.5426	-0.0241
10	0	10	11	9	0	9	10	20525.5652	-0.01181
10	0	10	10	9	0	9	9	20525.5652	-0.00492
10	0	10	9	9	0	9	8	20525.5652	0.00376
9	2	7	8	8	2	6	7	21155.2287	-0.02998
9	2	7	9	8	2	6	8	21155.2287	0.00804
9	2	7	10	8	2	6	9	21155.2287	-0.04283
10	2	9	11	9	2	8	10	21782.9034	-0.03778
10	2	9	10	9	2	8	9	21782.9034	-0.00093
10	2	9	9	9	2	8	8	21782.9034	-0.02693
11	1	11	12	10	1	10	11	22434.6724	-0.03246
11	1	11	11	10	1	10	10	22434.6724	-0.02219
12	0	12	13	11	0	11	12	24435.738	-0.00826
12	0	12	12	11	0	11	11	24435.738	-0.00175
12	0	12	11	11	0	11	10	24435.738	0.00234

S5.4 Measured frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}4$ CHT-1-CN-1 in the low-frequency region (2-26 GHz) fit using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	F	J'	K'_a	K'_c	F'	Observed Freq. (MHz)	Residuals (MHz)
2	1	2	2	1	1	1	1	4179.5271	0.00073
2	1	2	2	1	1	1	2	4180.179	0.00509
2	1	2	1	1	1	1	1	4180.5767	0.00871
2	1	2	3	1	1	1	2	4180.8628	0.01996
2	0	2	2	1	0	1	2	4415.0795	0.00965
2	0	2	1	1	0	1	0	4415.2697	-0.00141
2	0	2	2	1	0	1	1	4416.3427	0.0007
2	0	2	3	1	0	1	2	4416.4245	-0.00142
2	0	2	1	1	0	1	1	4418.4536	0.00167
2	1	1	2	1	1	0	1	4691.6841	-0.00168
2	1	1	2	1	1	0	2	4692.3105	0.00056
2	1	1	1	1	1	0	1	4692.7631	-0.00276
2	1	1	3	1	1	0	2	4693.007	0.00317
2	1	1	1	1	1	0	0	4694.3268	0.00012
3	1	3	3	2	1	2	3	6257.7072	0.00152
3	1	3	3	2	1	2	2	6258.3772	0.00256
3	1	3	2	2	1	2	1	6258.7514	0.00693
3	1	3	4	2	1	2	3	6258.7514	0.00063

3	1	3	2	2	1	2	2	6259.7854	-0.00063
3	0	3	3	2	0	2	3	6573.1676	0.00083
3	0	3	2	2	0	2	1	6574.2974	-0.00004
3	0	3	4	2	0	2	3	6574.5536	-0.00893
3	0	3	3	2	0	2	2	6574.5536	0.03082
3	0	3	2	2	0	2	2	6576.4101	0.00264
3	2	2	2	2	2	1	2	6653.9365	0.00435
3	2	2	2	2	2	1	3	6655.3004	0.00519
3	2	2	2	2	2	1	1	6656.0544	0.00206
3	2	1	3	2	2	0	2	6734.3995	-0.00602
3	2	1	2	2	2	0	3	6735.7766	-0.00941
3	2	1	2	2	2	0	1	6736.5303	-0.00888
3	1	2	3	2	1	1	3	7024.9008	-0.00586
3	1	2	3	2	1	1	2	7025.5984	-0.00212
3	1	2	2	2	1	1	1	7025.9727	0.00662
3	1	2	4	2	1	1	3	7025.9727	-0.00451
3	1	2	2	2	1	1	2	7027.0438	-0.00235
4	1	4	4	3	1	3	3	8323.2668	0.00038
4	1	4	5	3	1	3	4	8323.4278	-0.00397
4	1	4	3	3	1	3	2	8323.4278	0.05072
4	0	4	3	3	0	3	2	8677.208	0.00078
4	0	4	4	3	0	3	3	8677.3356	0.02239
4	0	4	5	3	0	3	4	8677.3356	0.00354
4	2	3	4	3	2	2	4	8857.0686	0.01111

4	2	3	5	3	2	2	4	8857.6433	0.00931
4	2	3	3	3	2	2	2	8857.7972	0.01509
4	2	2	4	3	2	1	3	9053.0149	-0.00995
4	2	2	5	3	2	1	4	9053.6005	-0.01422
4	1	3	3	3	1	2	2	9341.6878	0.04729
4	1	3	5	3	1	2	4	9341.6878	-0.00987
8	1	7	7	7	1	6	6	18242.3917	0.03442
8	1	7	9	7	1	6	8	18242.3917	0.01068
8	1	7	8	7	1	6	7	18242.3917	0.02525
9	1	9	8	8	1	8	7	18415.813	0.01364
9	1	9	10	8	1	8	9	18415.813	-0.00443
9	1	9	9	8	1	8	8	18415.813	0.01279
9	0	9	9	8	0	8	8	18534.6185	0.01688
9	0	9	8	8	0	8	7	18534.6185	0.03057
9	0	9	10	8	0	8	9	18534.6185	0.01088
8	2	6	8	7	2	5	7	18638.2304	0.08833
8	2	6	9	7	2	5	8	18638.2304	0.00981
8	2	6	7	7	2	5	6	18638.2304	0.02242
9	2	8	9	8	2	7	8	19611.2328	0.02285
9	2	8	8	8	2	7	7	19611.2328	-0.01739
9	2	8	10	8	2	7	9	19611.2328	-0.02914
9	1	8	10	8	1	7	9	20323.8134	0.00774
9	1	8	8	8	1	7	7	20323.8134	0.02712
9	1	8	9	8	1	7	8	20323.8134	0.01372

10	1	10	9	9	1	9	8	20397.7269	0.01247
10	1	10	10	9	1	9	9	20397.7269	0.0107
10	1	10	11	9	1	9	10	20397.7269	-0.00234
10	0	10	10	9	0	9	9	20475.5201	-0.0397
10	0	10	9	9	0	9	8	20475.5201	-0.03055
10	0	10	11	9	0	9	10	20475.5201	-0.0462
9	2	7	9	8	2	6	8	21009.8335	0.01903
9	2	7	8	8	2	6	7	21009.8335	-0.02037
9	2	7	10	8	2	6	9	21009.8335	-0.03307
10	2	9	10	9	2	8	9	21695.651	0.00927
10	2	9	9	9	2	8	8	21695.651	-0.01713
10	2	9	11	9	2	8	10	21695.651	-0.02797
10	1	9	9	9	1	8	8	22338.5653	-0.00275
10	1	9	11	9	1	8	10	22338.5653	-0.01869
10	1	9	10	9	1	8	9	22338.5653	-0.01774
11	1	11	10	10	1	10	9	22372.8477	-0.04136
11	1	11	12	10	1	10	11	22372.8477	-0.0537
11	1	11	11	10	1	10	10	22372.8477	-0.04343
11	0	11	11	10	0	10	10	22422.2784	0.05102
11	0	11	10	10	0	10	9	22422.2784	0.05724
11	0	11	12	10	0	10	11	22422.2784	0.04448
10	2	8	10	9	2	7	9	23336.3892	-0.01208
10	2	8	9	9	2	7	8	23336.3892	-0.03437
10	2	8	11	9	2	7	10	23336.3892	-0.04629

11	2	10	11	10	2	9	10	23756.9559	0.00843
11	2	10	10	10	2	9	9	23756.9559	-0.00915
11	2	10	12	10	2	9	11	23756.9559	0.00843

S5.5 Measured frequencies and residuals (in MHz) for the rotational transitions of $^{13}\text{C}8$ CHT-1-CN-1 in the low-frequency region (2-26 GHz) fit using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	F	J'	K'_a	K'_c	F'	Observed Freq. (MHz)	Residuals (MHz)
2	1	2	2	1	1	1	1	4179.8228	0.00261
2	1	2	1	1	1	1	1	4180.8635	0.00342
2	1	2	3	1	1	1	2	4181.1348	0.00019
2	1	2	1	1	1	1	0	4182.4697	-0.00682
2	0	2	2	1	0	1	2	4414.7223	-0.00501
2	0	2	1	1	0	1	0	4414.9244	-0.004
2	0	2	2	1	0	1	1	4415.9999	0.00243
2	0	2	3	1	0	1	2	4416.0793	-0.00209
2	1	1	2	1	1	0	1	4690.2022	0.00457
2	1	1	3	1	1	0	2	4691.5117	-0.00188
2	1	1	1	1	1	0	0	4692.8176	-0.01679
3	1	3	3	2	1	2	2	6258.9624	-0.00009
3	1	3	4	2	1	2	3	6259.3363	-0.00171
3	1	3	2	2	1	2	1	6259.3363	0.00456
3	0	3	3	2	0	2	3	6573.2574	-0.00535
3	0	3	2	2	0	2	1	6574.3861	-0.00593
3	0	3	3	2	0	2	2	6574.6385	0.02175
3	0	3	4	2	0	2	3	6574.6385	-0.01811

3	0	3	2	2	0	2	2	6576.4951	-0.00373
3	2	2	3	2	2	1	2	6653.0379	0.00276
3	2	2	4	2	2	1	3	6654.3982	0.00225
3	2	2	2	2	2	1	1	6655.1681	0.01572
3	2	1	3	2	2	0	2	6732.5111	-0.0056
3	2	1	4	2	2	0	3	6733.8912	0.00309
3	2	1	2	2	2	0	1	6734.6387	-0.00812
3	1	2	3	2	1	1	3	7022.824	-0.0204
3	1	2	3	2	1	1	2	7023.5243	-0.01295
3	1	2	4	2	1	1	3	7023.9032	-0.01018
3	1	2	2	2	1	1	1	7023.9032	0.00092
3	1	2	2	2	1	1	2	7024.978	-0.00273
4	1	4	4	3	1	3	3	8324.2869	-0.01249
4	1	4	3	3	1	3	2	8324.4616	0.05159
4	1	4	5	3	1	3	4	8324.4616	-0.003
4	0	4	3	3	0	3	2	8678.3301	-0.01016
4	0	4	4	3	0	3	3	8678.4584	0.01241
4	0	4	5	3	0	3	4	8678.4584	-0.0066
4	2	3	4	3	2	2	3	8856.0642	0.00528
4	2	3	5	3	2	2	4	8856.6385	0.00387
4	2	3	3	3	2	2	2	8856.7871	0.00452
4	1	3	4	3	1	2	3	9339.1263	-0.00557
4	1	3	5	3	1	2	4	9339.28	-0.01643
8	1	7	7	7	1	6	6	18243.8831	0.01738

8	1	7	8	7	1	6	7	18243.8831	0.00846
8	1	7	9	7	1	6	8	18243.8831	-0.0063
9	1	9	8	8	1	8	7	18420.7843	0.00219
9	1	9	10	8	1	8	9	18420.7843	-0.01585
9	1	9	9	8	1	8	8	18420.7843	0.00136
9	0	9	10	8	0	8	9	18541.697	0.00513
9	0	9	9	8	0	8	8	18541.697	0.01104
9	0	9	8	8	0	8	7	18541.697	0.02481
8	2	6	8	7	2	5	7	18630.3016	0.08738
8	2	6	9	7	2	5	8	18630.3016	0.00881
8	2	6	7	7	2	5	6	18630.3016	0.02138
9	1	8	9	8	1	7	8	20328.0887	0.01344
9	1	8	10	8	1	7	9	20328.0887	0.00726
9	1	8	8	8	1	7	7	20328.0887	0.02659
9	2	7	10	8	2	6	9	21002.514	-0.03375
9	2	7	9	8	2	6	8	21002.514	0.01848
9	2	7	8	8	2	6	7	21002.514	-0.0211
11	2	10	12	10	2	9	11	23760.9107	-0.0305
11	2	10	11	10	2	9	10	23760.9107	-0.0032
11	2	10	10	10	2	9	9	23760.9107	-0.0208
9	2	8	10	8	2	7	9	19611.2328	-0.02914
9	1	8	10	8	1	7	9	20323.8134	0.00774
9	1	8	8	8	1	7	7	20323.8134	0.02712
9	1	8	9	8	1	7	8	20323.8134	0.01372

10	1	10	9	9	1	9	8	20397.7269	0.01247
10	1	10	10	9	1	9	9	20397.7269	0.0107
10	1	10	11	9	1	9	10	20397.7269	-0.00234
10	0	10	10	9	0	9	9	20475.5201	-0.0397
10	0	10	9	9	0	9	8	20475.5201	-0.03055
10	0	10	11	9	0	9	10	20475.5201	-0.0462
9	2	7	9	8	2	6	8	21009.8335	0.01903
9	2	7	8	8	2	6	7	21009.8335	-0.02037
9	2	7	10	8	2	6	9	21009.8335	-0.03307
10	2	9	10	9	2	8	9	21695.651	0.00927
10	2	9	9	9	2	8	8	21695.651	-0.01713
10	2	9	11	9	2	8	10	21695.651	-0.02797
10	1	9	9	9	1	8	8	22338.5653	-0.00275
10	1	9	11	9	1	8	10	22338.5653	-0.01869
10	1	9	10	9	1	8	9	22338.5653	-0.01774
11	1	11	10	10	1	10	9	22372.8477	-0.04136
11	1	11	12	10	1	10	11	22372.8477	-0.0537
11	1	11	11	10	1	10	10	22372.8477	-0.04343
11	0	11	11	10	0	10	10	22422.2784	0.05102
11	0	11	10	10	0	10	9	22422.2784	0.05724
11	0	11	12	10	0	10	11	22422.2784	0.04448
10	2	8	10	9	2	7	9	23336.3892	-0.01208
10	2	8	9	9	2	7	8	23336.3892	-0.03437
10	2	8	11	9	2	7	10	23336.3892	-0.04629

11	2	10	11	10	2	9	10	23756.9559	0.00843
11	2	10	10	10	2	9	9	23756.9559	-0.00915
11	2	10	12	10	2	9	11	23756.9559	0.00843

S5.6 Measured frequencies and residuals (in MHz) for the rotational transitions of $^{15}\text{N}7$ CHT-1-CN-1 in the low-frequency region (2-26 GHz) fit using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	J'	K'_a	K'_c	Observed Freq. (MHz)	Residuals (MHz)
2	0	2	1	0	1	4355.9586	-0.0009
2	1	1	1	1	0	4623.1644	-0.0012
3	1	3	2	1	2	6178.4109	0.0047
3	0	3	2	0	2	6487.4315	0.0035
3	2	2	2	2	1	6562.2766	0.0108
3	2	1	2	2	0	6637.1122	0.0036
3	1	2	2	1	1	6922.4565	0.001
4	0	4	3	0	3	8567.032	-0.0004
8	1	7	7	1	6	18005.2693	0.0079
9	0	9	8	0	8	18321.967	0.0218
8	2	6	7	2	5	18352.4103	-0.0015
9	1	8	8	1	7	20071.631	-0.0129
10	1	10	9	1	9	20154.7048	-0.0196

**S6.0 The experimental and theoretical rotational constants for
the observed six low-lying vibrationally excited states of
CHT-1-CN-1.**

The experimental and theoretical rotational constants for the observed six low-lying vibrationally excited states of CHT-1-CN-1. The rotational constants A_{theory} , B_{theory} , and C_{theory} were corrected by 23.37 MHz, -4.14 MHz, and -3.85 MHz, respectively, to account for the differences in the experimental and theoretical rotational constants of the vibronic ground state. E_h and E_a are the harmonic and anharmonic energies of the vibrational states.

Vibrationally excited states of CHT-1-CN-1						
Rotational parameters	ν_{42}	ν_{41}	$2\nu_{42}$	$\nu_{42} + \nu_{41}$	ν_{40}	ν_{38}
E_h / cm^{-1}	110.2	149.4	220.4	259.9	271.3	320.4
E_a / cm^{-1}	110.4	145.8	219.9	255.4	269.8	318.3
Boltzmann population (%)	18.25	15.41	10.77	9.08	8.47	6.84
$A_{theory}^a / \text{MHz}$	3513.36	3565.02	3488.57	3540.26	3543.4	3537.92
$B_{theory}^b / \text{MHz}$	1251.37	1253.11	1251.34	1253.08	1251.25	1251.97
$C_{theory}^c / \text{MHz}$	990.65	991.04	990.68	991.07	990.14	990.26
A/MHz	3511.3491(46)	3565.8196(44)	3490.087(64)	3540.123(25)	3542.25(51)	3475.10(99)
B/MHz	1251.3275(32)	1253.2530(43)	1250.9389(69)	1251.7762(26)	1251.322(120)	1250.171(105)
C/MHz	990.57016(28)	991.31445(24)	990.50584(42)	990.21198(40)	990.13710(38)	990.416978(122)
Δ_j^b / kHz	0.055728(49)	0.056761(74)	0.056988(89)	0.055413(90)	0.054706(69)	0.057163(58)
$\Delta_{JK}^d / \text{kHz}$	0.15257(23)	0.2491(11)	0.123(16)	0.384(18)	0.384(18)	[0.20088039]
Δ_K^e / kHz	[0.83]	[0.83]	[0.83]	[0.83]	[0.83]	[0.766306647]
δ_j^f / kHz	-0.006529(36)	-0.007072(45)	[-0.006736]	[-0.006736]	[-0.006736]	[0.006736]
δ_K^f / kHz	-0.2151(13)	-0.3439(14)	-0.2002(84)	-0.3828(94)	-0.3828(94)	[0.277093198]
σ^g / kHz	92	120	112	100	150	76
No. of lines	714	361	123	107	63	96
J/K_a^d	54/31	54/13	54/6	47/4	47/4	44/3

^a A , B , and C are the rotational constants.

^b Δ_J , Δ_{JK} , Δ_K , δ_J , and δ_J are the quartic centrifugal distortion constants.

^c Microwave root-mean-square deviation of the fit.

^d Maximum values of J and K_a assigned in the fit.

S7.0 The list of assigned transitions for the observed six low-lying vibrationally excited states of CHT-1-CN-1.

S7.1 Measured frequencies and residuals (in MHz) for the rotational transitions of the vibrationally excited state ν_{42} of CHT-1-CN-1 in the frequency range of 75-110 GHz using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	J'	K'_a	K'_c	Observed Freq. (MHz)	Residuals (MHz)
33	12	22	32	12	21	75005.8023	0.0647
33	12	21	32	12	20	75005.8023	-0.0624
33	5	28	32	5	27	75047.4958	-0.0816
35	4	32	34	4	31	75059.2475	-0.004
35	3	32	34	3	31	75062.0183	0.033
33	11	23	32	11	22	75193.829	-0.0175
33	11	22	32	11	21	75195.769	-0.0789
36	2	34	35	2	33	75382.499	-0.0462
36	3	34	35	3	33	75382.499	0.0257
33	10	24	32	10	23	75446.41	0.0128
37	1	36	36	1	35	75729.082	0.0495
32	7	25	31	7	24	75842.059	-0.1133
33	8	26	32	8	25	75922.9843	-0.145

33	9	24	32	9	23		75966.088	-0.039
38	0	38	37	0	37		76085.064	0.0594
34	6	29	33	6	28		76416.9096	-0.0117
34	29	5	33	29	4		76493.4739	-0.0291
34	29	6	33	29	5		76493.4739	-0.0291
34	27	8	33	27	7		76520.4971	-0.0345
34	27	7	33	27	6		76520.4971	-0.0345
34	26	9	33	26	8		76536.3423	0.0485
34	26	8	33	26	7		76536.3423	0.0485
34	23	11	33	23	10		76595.9868	0.0491
34	23	12	33	23	11		76595.9868	0.0491
34	22	12	33	22	11		76621.2582	-0.0087
34	22	13	33	22	12		76621.2582	-0.0087
34	20	15	33	20	14		76683.609	-0.0056
34	20	14	33	20	13		76683.609	-0.0056
34	19	16	33	19	15		76722.431	0.0437
34	19	15	33	19	14		76722.431	0.0437
35	5	31	34	5	30		76748.6586	-0.012
34	18	16	33	18	15		76767.8475	0.0113
35	4	31	34	4	30		76786.9383	-0.0223
34	17	17	33	17	16		76821.7436	0.0863
34	16	18	33	16	17		76886.2269	0.0876
34	5	29	33	5	28		76892.1396	-0.0826
34	15	20	33	15	19		76964.448	0.0014

34	15	19	33	15	18	76964.448	0.0014
36	4	33	35	4	32	77036.2437	0.0362
36	3	33	35	3	32	77037.873	0.0142
34	14	20	33	14	19	77061.048	-0.0372
34	14	21	33	14	20	77061.048	-0.0365
33	8	25	32	8	24	77096.5286	-0.0165
34	13	22	33	13	21	77182.6628	-0.049
34	13	21	33	13	20	77182.6628	-0.0629
37	2	35	36	2	34	77361.92	-0.0059
34	11	24	33	11	23	77547.6235	-0.0277
34	7	28	33	7	27	77696.728	-0.0522
38	1	37	37	1	36	77709.277	0.0249
34	10	25	33	10	24	77824.276	-0.0211
34	10	24	33	10	23	77865.7816	-0.0431
39	0	39	38	0	38	78065.429	0.0583
34	9	26	33	9	25	78135.686	0.0057
34	8	27	33	8	26	78237.0973	-0.0224
33	7	26	32	7	25	78377.6756	-0.0225
35	6	30	34	6	29	78424.5286	-0.0269
36	5	32	35	5	31	78723.6229	-0.0219
36	4	32	35	4	31	78748.0731	-0.0143
35	5	30	34	5	29	78760.7796	-0.0144
35	27	8	34	27	7	78782.4612	0.0028
35	26	9	34	26	8	78799.6194	0.0026

35	25	10	34	25	9		78818.7565	-0.023
35	23	12	34	23	11		78864.6127	0.0169
35	23	13	34	23	12		78864.6127	0.0169
35	22	13	34	22	12		78892.2809	0.0708
35	22	14	34	22	13		78892.2809	0.0708
35	21	14	34	21	13		78923.8424	0.0379
35	21	15	34	21	14		78923.8424	0.0379
35	19	16	34	19	15		79002.5532	0.0103
35	19	17	34	19	16		79002.5532	0.0103
37	4	34	36	4	33		79013.377	-0.0011
37	3	34	36	3	33		79014.38	0.0105
35	18	18	34	18	17		79052.1442	-0.0319
35	18	17	34	18	16		79052.1442	-0.0319
35	17	19	34	17	18		79111.0139	0.0257
35	17	18	34	17	17		79111.0139	0.0257
35	16	19	34	16	18		79181.5162	0.0115
35	16	20	34	16	19		79181.5162	0.0115
35	15	20	34	15	19		79267.234	0.0047
35	15	21	34	15	20		79267.234	0.0047
38	2	36	37	2	35		79341.421	0.0429
35	14	21	34	14	20		79373.1538	-0.0223
35	14	22	34	14	21		79373.1538	-0.0209
34	6	28	33	6	27		79486.7795	-0.0542
35	13	23	34	13	22		79506.818	0.0208

35	13	22	34	13	21		79506.818	-0.0082
39	1	38	38	1	37		79689.494	0.0435
39	2	38	38	2	37		79689.494	0.0438
35	7	29	34	7	28		79820.2081	-0.0094
35	11	25	34	11	24		79909.189	0.0222
35	11	24	34	11	23		79915.898	0.0355
40	0	40	39	0	39		80045.77	0.0716
35	10	26	34	10	25		80209.503	-0.015
35	10	25	34	10	24		80278.78	0.0697
36	6	31	35	6	30		80419.811	-0.0078
35	9	27	34	9	26		80516.802	-0.0309
35	8	28	34	8	27		80524.71	-0.018
36	5	31	35	5	30		80652.575	0.0323
37	5	33	36	5	32		80697.8167	-0.0328
37	4	33	36	4	32		80713.304	-0.0006
34	7	27	33	7	26		80815.4213	-0.0877
38	3	35	37	3	34		80991.3087	-0.0567
35	9	26	34	9	25		81017.1372	-0.0277
36	28	8	35	28	7		81028.6496	0.0422
36	27	10	35	27	9		81045.4331	0.06
36	27	9	35	27	8		81045.4331	0.06
36	26	10	35	26	9		81064.0312	0.0212
36	26	11	35	26	10		81064.0312	0.0212
36	25	11	35	25	10		81084.7881	-0.0435

36	25	12	35	25	11		81084.7881	-0.0435
36	24	12	35	24	11		81108.2852	0.0658
36	24	13	35	24	12		81108.2852	0.0658
36	23	13	35	23	12		81134.6364	-0.0052
36	23	14	35	23	13		81134.6364	-0.0052
36	22	14	35	22	13		81164.7038	0.025
36	22	15	35	22	14		81164.7038	0.025
36	21	15	35	21	14		81199.1128	0.0548
36	21	16	35	21	15		81199.1128	0.0548
36	20	17	35	20	16		81238.753	0.0521
36	20	16	35	20	15		81238.753	0.0521
36	19	17	35	19	16		81284.8122	0.0209
36	19	18	35	19	17		81284.8122	0.0209
39	2	37	38	2	36		81320.917	0.0321
35	6	29	34	6	28		81330.6319	-0.077
36	18	18	35	18	17		81338.9223	0.0484
36	17	20	35	17	19		81402.992	-0.0077
36	17	19	35	17	18		81402.992	-0.0077
36	16	20	35	16	19		81479.9024	-0.0498
36	15	21	35	15	20		81573.6371	0.0302
36	15	22	35	15	21		81573.6371	0.0303
40	1	39	39	1	38		81669.647	0.0224
40	2	39	39	2	38		81669.647	0.0226
36	14	22	35	14	21		81689.5368	-0.0041

36	14	23	35	14	22		81689.5368	-0.0011
36	13	24	35	13	23		81836.117	0.024
36	13	23	35	13	22		81836.117	-0.0353
36	7	30	35	7	29		81912.531	-0.01
41	0	41	40	0	40		82026.052	0.0654
36	11	25	35	11	24		82290.495	0.014
37	6	32	36	6	31		82405.959	-0.0161
37	5	32	36	5	31		82564.156	0.0103
36	10	27	35	10	26		82600.958	-0.0205
38	5	34	37	5	33		82671.77	-0.0213
38	4	34	37	4	33		82681.467	-0.0132
36	10	26	35	10	25		82713.501	-0.0636
36	8	29	35	8	28		82781.925	-0.0127
36	6	30	35	6	29		83134.176	-0.0286
35	7	28	34	7	27		83141.499	-0.0484
37	31	7	36	31	6		83246.2887	0.0313
37	29	8	36	29	7		83274.7245	-0.0027
40	2	38	39	2	37		83300.463	0.0303
37	27	11	36	27	10		83309.333	0.0283
37	27	10	36	27	9		83309.333	0.0283
37	24	13	36	24	12		83377.4702	0.0215
37	24	14	36	24	13		83377.4702	0.0215
37	23	14	36	23	13		83406.129	0.0115
37	23	15	36	23	14		83406.129	0.0115

37	22	15	36	22	14		83438.7647	0.0447
37	22	16	36	22	15		83438.7647	0.0447
37	21	17	36	21	16		83476.0567	0.0072
37	21	16	36	21	15		83476.0567	0.0072
37	20	17	36	20	16		83519.1514	0.0395
37	20	18	36	20	17		83519.1514	0.0395
37	19	18	36	19	17		83569.2213	0.0197
37	19	19	36	19	18		83569.2213	0.0197
36	9	27	35	9	26		83618.3697	0.0214
37	18	20	36	18	19		83628.0205	0.011
37	18	19	36	18	18		83628.0205	0.011
41	1	40	40	1	39		83649.8001	0.0284
41	2	40	40	2	39		83649.8001	0.0285
37	17	20	36	17	19		83697.841	0.054
37	16	21	36	16	20		83781.6075	0.0097
37	16	22	36	16	21		83781.6075	0.0098
37	15	22	36	15	21		83883.732	0.0061
42	1	42	41	1	41		84006.324	0.0899
42	0	42	41	0	41		84006.324	0.0899
37	14	23	36	14	22		84010.371	-0.0033
37	13	24	36	13	23		84170.948	-0.0374
37	12	26	36	12	25		84379.7823	0.086
37	12	25	36	12	24		84381.413	-0.0332
38	6	33	37	6	32		84385.73	-0.0089

38	5	33	37	5	32		84491.573	-0.0223
39	5	35	38	5	34		84645.771	-0.0148
39	4	35	38	4	34		84651.7677	-0.0449
37	11	27	36	11	26		84656.259	0.0218
37	6	31	36	6	30		84926.667	-0.0175
40	4	37	39	4	36		84946.273	0.0724
37	10	28	36	10	27		84996.935	-0.0269
37	8	30	36	8	29		85005.847	0.0125
37	10	27	36	10	26		85175.886	0.055
36	8	28	35	8	27		85182.047	-0.0339
37	9	29	36	9	28		85249.822	0.0553
41	2	39	40	2	38		85280.032	0.0217
41	3	39	40	3	38		85280.032	0.0261
36	7	29	35	7	28		85347.9759	-0.0731
38	30	8	37	30	7		85520.7974	-0.008
38	30	9	37	30	8		85520.7974	-0.008
38	29	10	37	29	9		85536.8768	-0.0225
38	29	9	37	29	8		85536.8768	-0.0225
38	28	10	37	28	9		85554.5699	-0.07
38	28	11	37	28	10		85554.5699	-0.07
38	27	11	37	27	10		85574.2571	-0.0255
38	27	12	37	27	11		85574.2571	-0.0255
38	26	13	37	26	12		85596.1024	-0.0311
38	26	12	37	26	11		85596.1024	-0.0311

38	25	14	37	25	13		85620.5922	0.0291
38	25	13	37	25	12		85620.5922	0.0291
42	2	41	41	2	40		85629.926	0.0368
42	1	41	41	1	40		85629.926	0.0367
38	24	15	37	24	14		85647.97	-0.0524
38	24	14	37	24	13		85647.97	-0.0524
38	23	16	37	23	15		85679.1017	0.0359
38	23	15	37	23	14		85679.1017	0.0359
38	22	17	37	22	16		85714.3732	-0.0082
38	22	16	37	22	15		85714.3732	-0.0082
38	21	18	37	21	17		85754.8118	-0.0207
38	21	17	37	21	16		85754.8118	-0.0207
38	20	19	37	20	18		85801.5091	-0.0066
38	20	18	37	20	17		85801.5091	-0.0066
38	19	19	37	19	18		85855.8507	0.0071
38	19	20	37	19	19		85855.8507	0.0071
43	1	43	42	1	42		85986.514	0.0742
38	16	22	37	16	21		86086.5948	0.0321
38	16	23	37	16	22		86086.5948	0.0322
38	15	23	37	15	22		86197.724	-0.017
38	14	24	37	14	23		86335.867	-0.0174
39	6	34	38	6	33		86361.21	-0.0467
39	5	34	38	5	33		86431.1288	-0.0392
38	13	25	37	13	24		86511.5136	-0.1235

38	13	26	37	13	25		86511.5136	0.1067
40	5	36	39	5	35		86620.001	-0.0146
40	4	36	39	4	35		86623.741	0.0032
38	12	27	37	12	26		86740.342	-0.0569
38	12	26	37	12	25		86743.586	0.0025
41	3	38	40	3	37		86924.253	-0.0651
41	4	38	40	4	37		86924.253	0.0572
38	11	28	37	11	27		87041.9	0.0404
38	11	27	37	11	26		87076.44	0.0038
38	8	31	37	8	30		87194.822	0.0135
42	2	40	41	2	39		87259.5931	-0.0149
42	3	40	41	3	39		87259.5931	-0.0124
38	10	29	37	10	28		87394.997	-0.0066
37	7	30	36	7	29		87433.684	-0.0803
43	1	42	42	1	41		87610.008	0.0329
38	10	28	37	10	27		87672.2861	-0.0069
39	31	9	38	31	8		87766.77	-0.0609
39	31	8	38	31	7		87766.77	-0.0609
39	29	11	38	29	10		87800.035	0.04
39	29	10	38	29	9		87800.035	0.04
37	8	29	36	8	28		87805.937	0.0059
39	28	11	38	28	10		87819.1475	0.0119
39	28	12	38	28	11		87819.1475	0.0119
39	27	12	38	27	11		87840.3578	0.0219

39	27	13	38	27	12		87840.3578	0.0219
39	25	14	38	25	13		87890.3063	-0.0061
39	25	15	38	25	14		87890.3063	-0.0061
39	24	15	38	24	14		87920.0673	0.0882
39	24	16	38	24	15		87920.0673	0.0882
39	23	17	38	23	16		87953.5279	-0.0016
39	23	16	38	23	15		87953.5279	-0.0016
44	1	44	43	1	43		87966.675	0.0725
39	22	17	38	22	16		87991.7298	0.0191
39	22	18	38	22	17		87991.7298	0.0191
39	21	18	38	21	17		88035.4555	-0.0057
39	21	19	38	21	18		88035.4555	-0.0057
39	7	33	38	7	32		88036.4807	0.0287
39	20	19	38	20	18		88086.0072	0.033
39	20	20	38	20	19		88086.0072	0.033
39	19	20	38	19	19		88144.7813	-0.0078
39	19	21	38	19	20		88144.7813	-0.0078
39	18	21	38	18	20		88213.9176	-0.0081
39	18	22	38	18	21		88213.9176	-0.0081
39	17	22	38	17	21		88296.1235	0.0374
39	17	23	38	17	22		88296.1235	0.0374
40	6	35	39	6	34		88334.1551	0.0063
39	16	23	38	16	22		88394.9776	0.0044
39	16	24	38	16	23		88394.9776	0.0045

39	15	25	38	15	24		88515.818	0.0041
39	15	24	38	15	23		88515.818	0.0027
39	6	33	38	6	32		88556.448	-0.0359
41	5	37	40	5	36		88594.5369	-0.0385
41	4	37	40	4	36		88596.8327	-0.0265
39	14	26	38	14	25		88666.2876	0.0197
39	14	25	38	14	24		88666.2876	-0.0078
39	13	26	38	13	25		88858.4361	-0.0217
39	13	26	38	13	25		88858.4361	-0.0217
42	3	39	41	3	38		88902.388	-0.0341
42	4	39	41	4	38		88902.388	0.0376
38	9	29	37	9	28		88978.8275	-0.0549
39	12	28	38	12	27		89108.705	0.0317
39	12	27	38	12	26		89114.345	-0.0036
43	2	41	42	2	40		89239.219	0.0012
39	8	32	38	8	31		89348.646	0.0064
38	7	31	37	7	30		89405.9409	-0.038
39	11	29	38	11	28		89435.1411	-0.0136
39	11	28	38	11	27		89492.346	-0.0554
44	1	43	43	1	42		89590.05	0.0231
39	10	30	38	10	29		89791.812	-0.015
39	9	31	38	9	30		89908.7939	0.0176
45	0	45	44	0	44		89946.7829	0.0616
40	31	9	39	31	8		90028.32	-0.0204

40	31	10	39	31	9		90028.32	-0.0204
40	7	34	39	7	33		90039.9431	0.0114
40	30	10	39	30	9		90045.3619	0.0101
40	29	11	39	29	10		90064.0091	-0.0302
40	28	12	39	28	11		90084.5811	-0.0727
40	27	14	39	27	13		90107.451	-0.0433
40	27	13	39	27	12		90107.451	-0.0433
40	26	14	39	26	13		90132.89	-0.0298
40	25	16	39	25	15		90161.379	0.0144
40	25	15	39	25	14		90161.379	0.0144
40	24	17	39	24	16		90193.3594	0.0011
40	24	16	39	24	15		90193.3594	0.0011
39	10	29	38	10	28		90210.7394	-0.0358
40	23	18	39	23	17		90229.5599	0.0076
40	23	17	39	23	16		90229.5599	0.0076
40	22	19	39	22	18		90270.7697	0.0126
40	22	18	39	22	17		90270.7697	0.0126
41	6	36	40	6	35		90305.5441	-0.0413
40	21	20	39	21	19		90318.0558	0.0649
40	21	19	39	21	18		90318.0558	0.0649
41	5	36	40	5	35		90335.0406	-0.0337
40	20	21	39	20	20		90372.5775	0.0271
40	20	20	39	20	19		90372.5775	0.0271
40	6	34	39	6	33		90409.8236	0

40	19	22	39	19	21		90436.1092	-0.0026
40	19	21	39	19	20		90436.1092	-0.0026
40	18	23	39	18	22		90510.888	0.0102
40	18	22	39	18	21		90510.888	0.0102
42	5	38	41	5	37		90569.533	0.0298
42	4	38	41	4	37		90570.899	0.0029
40	16	24	39	16	23		90706.974	0.0125
40	16	25	39	16	24		90706.974	0.0126
59	2	57	59	2	58		90712.4852	0.1315
40	15	25	39	15	24		90838.1478	0.0258
40	15	26	39	15	25		90838.1478	0.0288
43	3	40	42	3	39		90880.642	-0.0433
43	4	40	42	4	39		90880.642	-0.0015
40	14	27	39	14	26		91001.839	0.0435
40	14	26	39	14	25		91001.839	-0.0111
44	2	42	43	2	41		91218.815	-0.0174
44	3	42	43	3	41		91218.815	-0.0167
39	7	32	38	7	31		91282.495	-0.0827
40	8	33	39	8	32		91468.3965	-0.0631
40	12	29	39	12	28		91484.7486	-0.0599
40	12	28	39	12	27		91494.7067	-0.0124
45	1	44	44	1	43		91570.046	0.0033
39	9	30	38	9	29		91713.9269	-0.0636
40	11	30	39	11	29		91835.337	-0.0076

46	1	46	45	1	45		91926.865	0.0701
40	11	29	39	11	28		91928.148	0.0083
41	7	35	40	7	34		92030.952	-0.0256
40	10	31	39	10	30		92183.3173	-0.0402
42	6	37	41	6	36		92276.349	-0.026
41	6	35	40	6	34		92288.7368	0.002
42	5	37	41	5	36		92295.1832	-0.0701
41	29	12	40	29	11		92329.0074	-0.0499
41	29	13	40	29	12		92329.0074	-0.0499
41	28	13	40	28	12		92351.2252	0.0035
41	28	14	40	28	13		92351.2252	0.0035
41	27	14	40	27	13		92375.7637	-0.0238
41	27	15	40	27	14		92375.7637	-0.0238
41	25	17	40	25	16		92433.7431	-0.0123
41	25	16	40	25	15		92433.7431	-0.0123
41	24	18	40	24	17		92468.194	-0.0051
41	24	17	40	24	16		92468.194	-0.0051
41	23	18	40	23	17		92507.1937	0.0155
41	23	19	40	23	18		92507.1937	0.0155
43	5	39	42	5	38		92544.811	0.0082
43	4	39	42	4	38		92545.69	0.0425
41	22	19	40	22	18		92551.5609	-0.0089
41	22	20	40	22	19		92551.5609	-0.0089
41	21	21	40	21	20		92602.4837	0.0061

41	21	20	40	21	19		92602.4837	0.0061
41	20	22	40	20	21		92661.3271	0.0179
41	20	21	40	20	20		92661.3271	0.0179
41	19	23	40	19	22		92729.8554	-0.0314
41	19	22	40	19	21		92729.8554	-0.0314
39	8	31	38	8	30		92769.1688	-0.0656
41	18	24	40	18	23		92810.635	0.0234
41	18	23	40	18	22		92810.635	0.0234
44	4	41	43	4	40		92859.0677	0.0125
44	3	41	43	3	40		92859.0677	-0.0119
41	17	25	40	17	24		92906.742	0.0258
41	17	24	40	17	23		92906.742	0.0258
41	16	25	40	16	24		93022.7024	0.0355
41	16	26	40	16	25		93022.7024	0.0358
40	7	33	39	7	32		93091.236	-0.0394
41	15	27	40	15	26		93164.852	0.0127
41	15	26	40	15	25		93164.852	0.0065
45	2	43	44	2	42		93198.4552	0.0095
45	3	43	44	3	42		93198.4552	0.0099
41	14	27	40	14	26		93342.781	-0.0333
41	14	28	40	14	27		93342.783	0.0753
46	1	45	45	1	44		93550.034	0.0132
41	8	34	40	8	33		93556.5693	-0.0287
41	12	30	40	12	29		93869.042	0.0394

41	12	29	40	12	28	93885.897	-0.0728
47	1	47	46	1	46	93906.882	0.0596
42	7	36	41	7	35	94012.868	-0.0352
42	6	36	41	6	35	94189.448	-0.0083
41	11	31	40	11	30	94241.133	0.0242
43	6	38	42	6	37	94247.038	-0.0117
43	5	38	42	5	37	94259.027	-0.0076
41	11	30	40	11	29	94388.2757	-0.0755
40	9	31	39	9	30	94450.1792	-0.059
41	9	33	40	9	32	94455.045	-0.0105
42	31	11	41	31	10	94553.8365	-0.0769
42	28	15	41	28	14	94618.8298	-0.0369
42	28	14	41	28	13	94618.8298	-0.0369
42	27	15	41	27	14	94645.2347	-0.0108
42	27	16	41	27	15	94645.2347	-0.0108
42	26	16	41	26	15	94674.646	0.0178
42	26	17	41	26	16	94674.646	0.0178
42	25	18	41	25	17	94707.5342	0.0132
42	25	17	41	25	16	94707.5342	0.0132
42	23	19	41	23	18	94786.4595	0.0078
42	23	20	41	23	19	94786.4595	0.0078
42	22	20	41	22	19	94834.189	-0.0102
42	22	21	41	22	20	94834.189	-0.0102
45	3	42	44	3	41	94837.577	-0.0049

41	7	34	40	7	33	94864.5063	-0.0098
42	21	22	41	21	21	94888.9986	0.0197
42	21	21	41	21	20	94888.9986	0.0197
42	19	23	41	19	22	95026.268	0.076
42	19	24	41	19	23	95026.268	0.076
40	8	32	39	8	31	95074.4997	-0.0671
42	18	25	41	18	24	95113.233	0.013
42	18	24	41	18	23	95113.233	0.013
46	2	44	45	2	43	95178.032	-0.0202
42	17	26	41	17	25	95216.947	0.0138
42	17	25	41	17	24	95216.947	0.0137
42	16	26	41	16	25	95342.2462	0.0104
42	16	27	41	16	26	95342.2462	0.011
42	15	27	41	15	26	95496.1845	0.0012
42	15	28	41	15	27	95496.1845	0.0138
47	1	46	46	1	45	95529.957	-0.0022
42	8	35	41	8	34	95616.306	-0.021
42	14	29	41	14	28	95689.353	0.0752
48	1	48	47	1	47	95886.861	0.0585
42	13	30	41	13	29	95937.5887	-0.0181
43	7	37	42	7	36	95988.454	-0.0115
43	6	37	42	6	36	96107.635	-0.0042
44	6	39	43	6	38	96217.951	0.0103
44	5	39	43	5	38	96225.51	0.0186

42	12	31	41	12	30	96261.3457	0.0438
42	12	30	41	12	29	96289.799	0.0073
42	7	35	41	7	34	96631.9835	-0.0215
42	11	32	41	11	31	96650.4594	-0.0001
42	9	34	41	9	33	96677.2074	-0.0084
46	3	43	45	3	42	96816.1759	0.003
46	4	43	45	4	42	96816.1759	0.0111
43	30	14	42	30	13	96838.945	-0.0766
43	30	13	42	30	12	96838.945	-0.0766
43	29	15	42	29	14	96862.0984	-0.0176
43	29	14	42	29	13	96862.0984	-0.0176
42	11	31	41	11	30	96879.0232	-0.0251
43	28	16	42	28	15	96887.6031	-0.0136
43	28	15	42	28	14	96887.6031	-0.0136
43	27	16	42	27	15	96915.854	-0.0442
43	27	17	42	27	16	96915.854	-0.0442
43	26	17	42	26	16	96947.4158	0.0056
43	26	18	42	26	17	96947.4158	0.0056
43	25	18	42	25	17	96982.6893	-0.0084
43	25	19	42	25	18	96982.6893	-0.0084
43	24	19	42	24	18	97022.4445	0.0178
43	24	20	42	24	19	97022.4445	0.0178
43	23	20	42	23	19	97067.4384	0.0202
43	23	21	42	23	20	97067.4384	0.0202

43	22	22	42	22	21		97118.7694	0.073
43	22	21	42	22	20		97118.7694	0.073
47	3	45	46	3	44		97157.6357	-0.0109
47	2	45	46	2	44		97157.6357	-0.011
43	21	23	42	21	22		97177.5803	0.0274
43	21	22	42	21	21		97177.5803	0.0274
43	20	23	42	20	22		97245.7064	0.0659
43	20	24	42	20	23		97245.7064	0.0659
43	19	24	42	19	23		97325.1408	0.0335
43	19	25	42	19	24		97325.1408	0.0335
43	18	26	42	18	25		97418.8583	0.0587
43	18	25	42	18	24		97418.8583	0.0587
48	2	47	47	2	46		97509.8507	-0.0057
48	1	47	47	1	46		97509.8507	-0.0057
43	8	36	42	8	35		97651.5451	0.0039
43	16	27	42	16	26		97665.8727	0.0493
43	16	28	42	16	27		97665.8727	0.0507
43	15	29	42	15	28		97832.3397	0.0167
43	15	28	42	15	27		97832.3397	-0.0085
49	0	49	48	0	48		97866.774	0.0397
49	0	49	48	0	48		97866.7753	0.041
49	1	49	48	1	48		97866.7753	0.041
44	7	38	43	7	37		97959.7967	-0.0527
43	14	30	42	14	29		98041.7171	-0.0811

43	14	29	42	14	28	98042.2387	0.0591
45	6	40	44	6	39	98189.2136	-0.0245
45	5	40	44	5	39	98193.975	0.0132
43	7	36	42	7	35	98414.9686	0.0127
46	5	42	45	5	41	98472.789	0.0644
46	4	42	45	4	41	98472.789	-0.1185
43	12	32	42	12	31	98661.5116	-0.0072
43	12	31	42	12	30	98708.4402	-0.0069
47	3	44	46	3	43	98794.807	-0.0295
43	9	35	42	9	34	98863.217	0.0344
43	11	33	42	11	32	99060.5879	-0.0576
44	30	15	43	30	14	99105.4671	-0.0317
44	30	14	43	30	13	99105.4671	-0.0317
44	29	15	43	29	14	99130.1268	-0.0808
44	29	16	43	29	15	99130.1268	-0.0808
48	2	46	47	2	45	99137.22	-0.005
44	28	16	43	28	15	99157.5273	0.028
44	28	17	43	28	16	99157.5273	0.028
44	27	18	43	27	17	99187.784	0.0078
44	27	17	43	27	16	99187.784	0.0078
44	26	19	43	26	18	99221.5094	-0.0125
44	26	18	43	26	17	99221.5094	-0.0125
44	25	20	43	25	19	99259.3566	0.0341
44	25	19	43	25	18	99259.3566	0.0341

43	10	34	42	10	33		99276.6763	0.0519
44	23	22	43	23	21		99350.1612	0.0375
44	23	21	43	23	20		99350.1612	0.0375
44	22	22	43	22	21		99405.1597	0.0462
44	22	23	43	22	22		99405.1597	0.0462
44	21	24	43	21	23		99468.2988	0.0391
44	21	23	43	21	22		99468.2988	0.0391
49	1	48	48	1	47		99489.753	0.0424
44	19	26	43	19	25		99626.7593	0.0442
44	19	25	43	19	24		99626.7593	0.0442
44	8	37	43	8	36		99666.428	0.0154
42	9	33	41	9	32		99782.3739	-0.0489
50	0	50	49	0	49		99846.6558	0.0391
44	17	28	43	17	27		99847.8081	0.0363
45	7	39	44	7	38		99928.7	-0.0096
45	6	39	44	6	38		99981.0709	0.008
46	6	41	45	6	40		100160.985	-0.0517
46	5	41	45	5	40		100163.98	0.0072
44	15	29	43	15	28		100173.591	0.0204
44	15	30	43	15	29		100173.591	0.0695
44	7	37	43	7	36		100224.568	0.0374
44	7	37	43	7	36		100224.568	0.0374
44	14	31	43	14	30		100400.564	-0.0166
47	4	43	46	4	42		100449.314	-0.0681

44	13	32	43	13	31		100693.887	0.0305
44	13	31	43	13	30		100702.04	-0.0234
48	4	45	47	4	44		100773.543	-0.0127
48	3	45	47	3	44		100773.543	-0.0154
43	10	33	42	10	32		100888.138	-0.0587
44	9	36	43	9	35		101013.042	0.0095
49	3	47	48	3	46		101116.762	-0.0207
49	2	47	48	2	46		101116.762	-0.0208
44	12	32	43	12	31		101144.91	-0.0552
45	31	14	44	31	13		101348.888	-0.0965
45	30	15	44	30	14		101372.877	-0.099
45	28	17	44	28	16		101428.52	-0.0227
50	1	49	49	1	48		101469.504	-0.0163
45	26	19	44	26	18		101497.004	0.0074
45	26	20	44	26	19		101497.004	0.0074
45	25	20	44	25	19		101537.454	0.0211
45	25	21	44	25	20		101537.454	0.0211
45	24	22	44	24	21		101583.025	0.0368
45	24	21	44	24	20		101583.025	0.0368
44	10	35	43	10	34		101596.405	-0.0141
45	23	23	44	23	22		101634.64	0.0249
45	23	22	44	23	21		101634.64	0.0249
45	22	24	44	22	23		101693.587	0.0837
45	22	23	44	22	22		101693.587	0.0837

45	21	24	44	21	23		101761.188	0.0275
45	21	25	44	21	24		101761.188	0.0275
51	0	51	50	0	50		101826.487	0.0386
51	1	51	50	1	50		101826.487	0.0386
45	20	25	44	20	24		101839.617	0.0993
45	20	26	44	20	25		101839.617	0.0993
46	7	40	45	7	39		101896.237	-0.0086
45	19	27	44	19	26		101931.132	0.0311
45	19	26	44	19	25		101931.132	0.0311
45	18	28	44	18	27		102039.317	0.0394
45	18	27	44	18	26		102039.317	0.0394
47	6	42	46	6	41		102133.387	0.0165
47	5	42	46	5	41		102135.164	-0.021
45	17	29	44	17	28		102168.716	0.064
45	17	28	44	17	27		102168.716	0.0637
45	16	29	44	16	28		102325.717	-0.0072
45	16	30	44	16	29		102325.717	-0.0014
48	4	44	47	4	43		102426.052	-0.0697
45	15	30	44	15	29		102520.048	-0.0545
45	15	31	44	15	30		102520.048	0.0394
49	3	46	48	3	45		102752.266	-0.0612
49	4	46	48	4	45		102752.266	-0.0596
50	3	48	49	3	47		103096.29	-0.0271
50	2	48	49	2	47		103096.29	-0.0272

45	13	32	44	13	31		103097.779	0.003
45	9	37	44	9	36		103128.214	0.0313
51	1	50	50	1	49		103449.291	0.0064
51	2	50	50	2	49		103449.291	0.0064
46	30	16	45	30	15		103641.45	-0.0268
46	29	17	45	29	16		103669.621	-0.0235
46	28	19	45	28	18		103700.757	-0.0175
46	28	18	45	28	17		103700.757	-0.0175
46	26	20	45	26	19		103773.862	-0.0078
46	26	21	45	26	20		103773.862	-0.0078
52	0	52	51	0	51		103806.261	0.0323
52	1	52	51	1	51		103806.261	0.0323
46	25	21	45	25	20		103817.073	0.0074
46	25	22	45	25	21		103817.073	0.0074
47	7	41	46	7	40		103863.33	0.0426
46	24	23	45	24	22		103865.765	0.0168
46	24	22	45	24	21		103865.765	0.0168
46	7	39	45	7	38		103930.641	-0.0351
46	22	24	45	22	23		103983.942	0.0213
46	22	25	45	22	24		103983.942	0.0213
46	21	26	45	21	25		104056.279	-0.0379
46	21	25	45	21	24		104056.279	-0.0379
48	6	43	47	6	42		104106.225	-0.0105
48	5	43	47	5	42		104107.328	-0.0228

46	20	26	45	20	25		104140.252	0.0363
46	20	27	45	20	26		104140.252	0.0363
46	19	28	45	19	27		104238.383	0.0299
46	19	27	45	19	26		104238.383	0.0299
46	18	28	45	18	27		104354.43	0.0392
46	18	29	45	18	28		104354.433	0.0427
46	18	28	45	18	27		104354.433	0.0426
49	4	45	48	4	44		104403.033	-0.0528
49	5	45	48	5	44		104403.033	-0.0148
46	17	30	45	17	29		104493.421	0.0655
46	17	29	45	17	28		104493.421	0.0648
45	11	34	44	11	33		104609.669	-0.0323
46	16	30	45	16	29		104662.357	-0.0449
46	16	31	45	16	30		104662.357	-0.0334
44	9	35	43	9	34		104726.297	-0.0487
50	3	47	49	3	46		104731.091	-0.04
50	4	47	49	4	46		104731.091	-0.0391
45	8	37	44	8	36		104848.46	0.0487
46	15	31	45	15	30		104872.13	-0.0896
46	15	32	45	15	31		104872.13	0.0869
51	3	49	50	3	48		105075.809	-0.0145
51	2	49	50	2	48		105075.809	-0.0145
46	14	33	45	14	32		105138.32	0.0613
46	14	33	45	14	32		105138.32	0.0613

52	1	51	51	1	50		105428.98	-0.0208
53	0	53	52	0	52		105785.987	0.0306
53	1	53	52	1	52		105785.987	0.0306
47	31	17	46	31	16		105883.691	-0.0714
47	31	16	46	31	15		105883.691	-0.0714
47	28	19	46	28	18		105974.211	-0.0132
47	28	20	46	28	19		105974.211	-0.0132
47	27	21	46	27	20		106011.036	-0.0337
47	27	20	46	27	19		106011.036	-0.0337
47	26	22	46	26	21		106052.161	-0.013
47	26	21	46	26	20		106052.161	-0.013
47	25	23	46	25	22		106098.272	0.0119
47	25	22	46	25	21		106098.272	0.0119
47	24	24	46	24	23		106150.227	0.0096
47	24	23	46	24	22		106150.227	0.0096
47	23	25	46	23	24		106209.118	-0.0272
47	23	24	46	23	23		106209.118	-0.0272
46	11	36	45	11	35		106256.971	0.0058
47	22	26	46	22	25		106276.467	0.0461
47	22	25	46	22	24		106276.467	0.0461
47	21	27	46	21	26		106353.858	0.0627
47	21	26	46	21	25		106353.858	0.0627
45	10	35	44	10	34		106419.855	-0.0313
47	20	27	46	20	26		106443.572	0.0508

47	20	28	46	20	27		106443.572	0.0508
47	19	28	46	19	27		106548.607	0.0424
47	19	29	46	19	28		106548.607	0.0424
46	8	38	45	8	37		106592.97	0.0366
47	18	30	46	18	29		106672.929	0.0266
47	18	29	46	18	28		106672.929	0.0265
51	3	48	50	3	47		106709.854	-0.1071
51	3	48	50	3	47		106709.873	-0.0883
51	4	48	50	4	47		106709.873	-0.0878
47	17	31	46	17	30		106822.051	0.0191
47	17	30	46	17	29		106822.051	0.0178
47	16	32	46	16	31		107003.863	0.0565
47	16	31	46	16	30		107003.863	0.034
45	9	36	44	9	35		107007.119	-0.0068
52	2	50	51	2	49		107055.256	-0.0441
52	3	50	51	3	49		107055.256	-0.0441
47	9	39	46	9	38		107265.639	0.041
53	1	52	52	1	51		107408.666	-0.0025
53	2	52	52	2	51		107408.666	-0.0025
47	14	34	46	14	33		107517.891	0.0547
47	14	33	46	14	32		107521.688	-0.0729
48	8	41	47	8	40		107599.54	0.0105
48	7	41	47	7	40		107730.423	-0.0009
54	1	54	53	1	53		107765.662	0.031

54	0	54	53	0	53		107765.662	0.031
49	7	43	48	7	42		107797.896	0.0188
49	6	43	48	6	42		107806.893	-0.0116
47	13	35	46	13	34		107888.117	0.0281
47	13	34	46	13	33		107926.239	-0.0261
50	6	45	49	6	44		108053.342	-0.1044
48	30	18	47	30	17		108181.604	-0.0412
48	29	20	47	29	19		108213.516	-0.0771
48	28	20	47	28	19		108248.903	-0.0177
48	27	22	47	27	21		108288.168	0.0094
48	27	21	47	27	20		108288.168	0.0094
47	12	36	46	12	35		108323.462	-0.0548
48	26	23	47	26	22		108331.926	-0.0186
48	26	22	47	26	21		108331.926	-0.0186
47	8	39	46	8	38		108337.135	0.0663
51	5	47	50	5	46		108357.526	-0.0191
51	4	47	50	4	46		108357.526	-0.0322
48	25	23	47	25	22		108381.057	0.0024
48	25	24	47	25	23		108381.057	0.0024
48	24	24	47	24	23		108436.447	0.0057
48	24	25	47	24	24		108436.447	0.0057
48	23	26	47	23	25		108499.317	0.0344
48	23	25	47	23	24		108499.317	0.0344
48	22	26	47	22	25		108571.094	0.0325

48	22	27	47	22	26		108571.094	0.0325
47	12	35	46	12	34		108608.063	-0.0118
47	11	37	46	11	36		108628.095	0.0122
52	3	49	51	3	48		108688.786	-0.0233
52	4	49	51	4	48		108688.786	-0.023
48	19	30	47	19	29		108861.841	0.0111
48	19	29	47	19	28		108861.841	0.0111
48	18	31	47	18	30		108994.966	0.0308
48	18	30	47	18	29		108994.966	0.0306
53	3	51	52	3	50		109034.71	-0.0327
53	2	51	52	2	50		109034.71	-0.0327
46	9	37	45	9	36		109151.861	0.0311
48	17	32	47	17	31		109154.886	0.0487
48	17	31	47	17	30		109154.886	0.0461
48	9	40	47	9	39		109295.429	0.0423
48	16	32	47	16	31		109350.288	0.0633
48	16	33	47	16	32		109350.288	0.1064
54	1	53	53	1	52		109388.295	0.0089
54	2	53	53	2	52		109388.295	0.0089

S7.2 Measured frequencies and residuals (in MHz) for the rotational transitions of the vibrationally excited state ν_{41} of CHT-1-CN-1 in the frequency range of 75-110 GHz using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	J'	K'_a	K'_c	Observed Freq. (MHz)	Residuals (MHz)
34	5	30	33	5	29	74919.6378	0.0124
33	13	20	32	13	19	74938.881	0.0252
33	13	21	32	13	20	74938.881	0.0305
34	4	30	33	4	29	74987.9157	0.0626
33	12	22	32	12	21	75079.0719	0.0235
33	12	21	32	12	20	75079.0719	-0.0825
35	4	32	34	4	31	75186.712	0.0229
33	11	23	32	11	22	75264.3587	-0.0092
33	5	28	32	5	27	75265.3544	0.0562
33	11	22	32	11	21	75266.0994	0.0294
36	3	34	35	3	33	75489.2723	0.0642
36	2	34	35	2	33	75489.2723	-0.0223
33	10	23	32	10	22	75534.6396	-0.0598
32	6	26	31	6	25	75741.3814	-0.0336
37	2	36	36	2	35	75815.8116	-0.0279
37	1	36	36	1	35	75815.8116	-0.0292

33	9	25	32	9	24		75818.7371	0.0006
32	7	25	31	7	24		75883.5731	-0.0497
33	8	26	32	8	25		76009.2421	-0.0485
38	0	38	37	0	37		76152.1097	-0.0666
38	1	38	37	1	37		76152.1097	-0.0666
34	6	29	33	6	28		76574.1412	0.0911
35	5	31	34	5	30		76898.3244	0.0517
35	4	31	34	4	30		76942.638	0.0255
33	8	25	32	8	24		77099.0321	-0.0858
36	4	33	35	4	32		77165.0663	0.0013
36	3	33	35	3	32		77167.0291	0.0046
34	13	22	33	13	21		77259.5501	0.0263
34	13	21	33	13	20		77259.5501	0.015
34	12	22	33	12	21		77414.2829	-0.1192
34	12	23	33	12	22		77414.2829	0.0926
37	3	35	36	3	34		77470.0967	0.0088
37	2	35	36	2	34		77470.0967	-0.0413
34	11	24	33	11	23		77619.0981	-0.0121
33	6	27	32	6	26		77782.5354	0.0856
38	2	37	37	2	36		77797.5444	-0.0095
38	1	37	37	1	36		77797.5444	-0.0102
34	7	28	33	7	27		77832.9421	-0.0062
34	10	25	33	10	24		77892.4645	0.043
34	10	24	33	10	23		77928.5721	-0.0164

39	0	39	38	0	38		78133.9891	-0.0458
39	1	39	38	1	38		78133.9891	-0.0458
34	9	26	33	9	25		78206.8973	-0.0468
34	8	27	33	8	26		78332.8754	-0.0531
33	7	26	32	7	25		78446.9019	-0.0182
34	9	25	33	9	24		78505.1492	-0.0216
35	6	30	34	6	29		78587.7243	0.0617
36	5	32	35	5	31		78875.1431	0.0525
37	4	34	36	4	33		79143.6291	-0.0177
37	3	34	36	3	33		79144.8638	0.033
38	3	36	37	3	35		79451.0572	0.0272
38	2	36	37	2	35		79451.0572	-0.0017
35	13	22	34	13	21		79585.0971	0.0033
35	13	23	34	13	22		79585.0971	0.0271
34	6	28	33	6	27		79723.7044	0.0904
35	12	24	34	12	23		79755.5744	0.1694
35	12	23	34	12	22		79755.5744	-0.2436
39	2	38	38	2	37		79779.2451	-0.0025
39	1	38	38	1	37		79779.2451	-0.0029
34	8	26	33	8	25		79792.2031	-0.0556
35	7	29	34	7	28		79968.1536	-0.0147
40	0	40	39	0	39		80115.8285	-0.0268
40	1	40	39	1	39		80115.8285	-0.0268
35	10	26	34	10	25		80278.7761	-0.0237

35	10	25	34	10	24		80339.178	-0.0253
36	6	31	35	6	30		80587.9131	0.0235
35	9	27	34	9	26		80592.7882	-0.0184
35	8	28	34	8	27		80631.6233	-0.0034
37	5	33	36	5	32		80850.9945	0.0569
36	5	31	35	5	30		80852.7576	0.0366
37	4	33	36	4	32		80869.1157	0.0305
34	7	27	33	7	26		80918.1593	0.0312
38	4	35	37	4	34		81122.4539	0.0015
38	3	35	37	3	34		81123.0832	-0.0804
39	3	37	38	3	36		81432.0529	0.0299
39	2	37	38	2	36		81432.0529	0.0133
35	6	29	34	6	28		81586.3203	0.0741
40	2	39	39	2	38		81760.91	-0.0079
40	1	39	39	1	38		81760.91	-0.0082
36	13	24	35	13	23		81915.7832	0.0523
36	13	23	35	13	22		81915.7832	0.0037
36	7	30	35	7	29		82071.6786	0.0038
41	1	41	40	1	40		82097.5933	-0.0429
41	0	41	40	0	40		82097.5933	-0.0429
36	12	25	35	12	24		82102.9372	-0.0866
36	12	24	35	12	23		82103.8182	0.0077
36	11	26	35	11	25		82351.6308	-0.0179
36	11	25	35	11	24		82361.7279	-0.0259

35	8	27	34	8	26		82503.9023	0.0419
37	6	32	36	6	31		82578.1151	0.0127
36	10	27	35	10	26		82671.7695	-0.006
37	5	32	36	5	31		82759.6965	0.0302
38	5	34	37	5	33		82826.4165	0.0288
38	4	34	37	4	33		82837.8907	0.0493
36	8	29	35	8	28		82901.1426	-0.0098
36	9	28	35	9	27		82972.0014	-0.0322
39	4	36	38	4	35		83101.7263	0.2475
39	3	36	38	3	35		83101.7263	-0.1776
39	4	36	38	4	35		83101.7263	0.2475
39	3	36	38	3	35		83101.7263	-0.1776
39	4	36	38	4	35		83101.7263	0.2475
39	3	36	38	3	35		83101.7263	-0.1776
36	6	30	35	6	29		83399.4069	0.0698
40	2	38	39	2	37		83413.0667	0.0012
40	3	38	39	3	37		83413.0667	0.0108
41	2	40	40	2	39		83742.5856	0.0238
41	1	40	40	1	39		83742.5856	0.0236
42	0	42	41	0	41		84079.3371	-0.0392
42	1	42	41	1	41		84079.3371	-0.0392
37	7	31	36	7	30		84146.2294	0.0059
37	13	25	36	13	24		84251.8616	0.096
37	13	24	36	13	23		84251.8616	-0.0009

38	6	33	37	6	32	84561.192	0.0361
38	5	33	37	5	32	84683.6808	0.0161
37	11	27	36	11	26	84729.8815	-0.0184
37	11	26	36	11	25	84747.3984	0.003
39	5	35	38	5	34	84801.8304	0.0245
39	4	35	38	4	34	84809.0084	0.0305
37	10	28	36	10	27	85069.7646	-0.0922
37	8	30	36	8	29	85138.2666	-0.0052
37	6	31	36	6	30	85193.0539	0.0321
36	8	28	35	8	27	85202.1056	-0.0243
37	10	27	36	10	26	85226.9058	-0.0544
37	9	29	36	9	28	85339.7009	-0.0348
41	3	39	40	3	38	85394.1474	0.028
41	2	39	40	2	38	85394.1474	0.0226
36	7	29	35	7	28	85527.3156	0.0496
42	1	41	41	1	40	85724.1806	0.0036
42	2	41	41	2	40	85724.1806	0.0036
43	0	43	42	0	42	86061.0403	-0.0345
43	1	43	42	1	42	86061.0403	-0.0345
38	7	32	37	7	31	86195.3065	-0.0222
37	9	28	36	9	27	86275.6968	-0.0248
39	6	34	38	6	33	86539.3631	0.0162
38	13	25	37	13	24	86593.5819	-0.0589
38	13	26	37	13	25	86593.5819	0.1302

39	5	34	38	5	33		86620.8953	0.0081
40	5	36	39	5	35		86777.4512	0.0409
40	4	36	39	4	35		86781.8754	0.0064
38	12	26	37	12	25		86821.5282	0.0012
38	6	32	37	6	31		86991.7258	0.0244
38	11	28	37	11	27		87116.2173	0.014
38	11	27	37	11	26		87145.8466	-0.008
38	8	31	37	8	30		87340.9951	0.0168
42	2	40	41	2	39		87375.2101	0.0027
42	3	40	41	3	39		87375.2101	0.0058
38	10	29	37	10	28		87470.8542	0.0034
37	7	30	36	7	29		87652.444	0.018
38	9	30	37	9	29		87690.6725	-0.0158
43	1	42	42	1	41		87705.772	0.0111
43	2	42	42	2	41		87705.772	0.0111
38	10	28	37	10	27		87715.4695	0.0945
37	8	29	36	8	28		87852.2453	-0.0144
44	0	44	43	0	43		88042.6765	-0.0538
44	1	44	43	1	43		88042.6765	-0.0538
39	7	33	38	7	32		88222.8999	-0.0305
40	6	35	39	6	34		88514.4205	-0.0187
40	5	35	39	5	34		88568.1042	0.0351
41	4	37	40	4	36		88756.08	0.0068
39	6	33	38	6	32		88810.4908	0.0411

39	13	27	38	13	26		88941.3442	0.2582
39	13	26	38	13	25		88941.3442	-0.1027
38	9	29	37	9	28		88970.7526	0.0102
42	3	39	41	3	38		89039.735	-0.0759
39	12	28	38	12	27		89187.811	0.0497
39	12	27	38	12	26		89192.5041	-0.0219
43	2	41	42	2	40		89356.3225	0.0175
43	3	41	42	3	40		89356.3225	0.0193
39	8	32	38	8	31		89508.5501	-0.0626
39	11	29	38	11	28		89510.3211	0.0152
39	11	28	38	11	27		89559.4883	-0.0281
38	7	31	37	7	30		89661.1961	0.04
44	2	43	43	2	42		89687.3201	0.0085
44	1	43	43	1	42		89687.3201	0.0085
39	10	30	38	10	29		89871.7464	-0.0357
39	9	31	38	9	30		90019.6424	-0.0317
45	1	45	44	1	44		90024.2651	-0.0767
40	7	34	39	7	33		90233.062	-0.0022
39	10	29	38	10	28		90243.0533	0.0085
38	8	30	37	8	29		90423.2395	-0.0258
41	6	36	40	6	35		90487.7577	0.0285
40	6	34	39	6	33		90655.4731	0.0029
42	5	38	41	5	37		90729.5887	0.0003
42	4	38	41	4	37		90731.3036	0.0251

43	3	40	42	3	39		91019.5186	0.0099
44	2	42	43	2	41		91337.4234	0.0136
44	3	42	43	3	41		91337.4234	0.0146
40	12	29	39	12	28		91564.3773	-0.03
39	7	32	38	7	31		91567.7034	0.0503
40	12	28	39	12	27		91572.7539	0.0119
40	8	33	39	8	32		91641.8279	-0.0359
45	2	44	44	2	43		91668.8335	0.0067
45	1	44	44	1	43		91668.8335	0.0067
39	9	30	38	9	29		91703.4054	0.0049
39	9	30	38	9	29		91703.4054	0.0049
40	11	30	39	11	29		91911.5854	-0.0025
40	11	29	39	11	28		91991.5467	-0.0322
46	1	46	45	1	45		92005.8647	-0.0434
46	0	46	45	0	45		92005.8647	-0.0434
41	7	35	40	7	34		92229.5415	-0.0335
40	10	31	39	10	30		92268.8159	-0.0642
40	9	32	39	9	31		92321.8434	-0.014
42	5	37	41	5	36		92482.5597	-0.0721
41	6	35	40	6	34		92526.7962	-0.0257
43	5	39	42	5	38		92706.2525	0.0228
43	4	39	42	4	38		92707.2944	0.0332
40	10	30	39	10	29		92817.9189	0.0362
39	8	31	38	8	30		92891.8344	0.0345

44	3	41	43	3	40	92999.3187	-0.0285
45	2	43	44	2	42	93318.5336	0.0179
45	3	43	44	3	42	93318.5336	0.0185
40	7	33	39	7	32	93396.493	0.0452
46	2	45	45	2	44	93650.2984	-0.0063
46	1	45	45	1	44	93650.2984	-0.0063
41	13	29	40	13	28	93655.5317	0.0544
41	13	28	40	13	27	93656.7279	0.0142
41	8	34	40	8	33	93742.5992	-0.056
41	12	30	40	12	29	93949.0839	0.0566
41	12	29	40	12	28	93963.2827	-0.041
47	0	47	46	0	46	93987.3864	-0.0419
47	1	47	46	1	46	93987.3864	-0.0419
42	7	36	41	7	35	94215.9222	0.0152
42	6	36	41	6	35	94421.37	0.0126
43	6	38	42	6	37	94432.3015	0.0501
43	5	38	42	5	37	94446.6119	-0.0245
40	9	31	39	9	30	94448.1022	0.058
41	9	33	40	9	32	94593.0724	-0.0743
41	10	32	40	10	31	94657.673	0.0166
44	5	40	43	5	39	94683.2802	0.0465
44	4	40	43	4	39	94683.8009	-0.059
45	3	42	44	3	41	94979.3239	0.022
41	7	34	40	7	33	95178.7898	-0.0138

40	8	32	39	8	31	95242.4987	0.0362
46	3	44	45	3	43	95299.6341	0.0176
46	2	44	45	2	43	95299.6341	0.0173
41	10	31	40	10	30	95446.6166	0.0653
47	1	46	46	1	45	95631.7704	0.0269
42	8	35	41	8	34	95813.88	-0.0482
48	0	48	47	0	47	95968.8686	-0.0325
48	1	48	47	1	47	95968.8686	-0.0325
42	13	29	41	13	28	96025.1695	0.0392
43	7	37	42	7	36	96194.928	-0.0549
43	6	37	42	6	36	96334.8159	-0.0248
42	12	31	41	12	30	96341.7441	0.0173
42	12	30	41	12	29	96365.7821	-0.0017
44	6	39	43	6	38	96404.4725	-0.0159
44	5	39	43	5	38	96413.5796	-0.0334
45	5	41	44	5	40	96660.5736	-0.0035
42	11	32	41	11	31	96730.591	-0.0515
42	9	34	41	9	33	96830.4836	-0.0132
42	11	31	41	11	30	96929.0882	-0.0097
42	7	35	41	7	34	96945.8193	0.0017
46	3	43	45	3	42	96959.3688	0.0164
42	10	33	41	10	32	97033.0852	-0.0001
47	3	45	46	3	44	97280.7493	0.0416
47	2	45	46	2	44	97280.7493	0.0414

41	8	33	40	8	32	97466.804	0.0366
48	1	47	47	1	46	97613.1533	0.0117
48	2	47	47	2	46	97613.1533	0.0117
43	8	36	42	8	35	97859.3744	0.0262
49	0	49	48	0	48	97950.3793	0.0537
49	1	49	48	1	48	97950.3793	0.0537
44	7	38	43	7	37	98169.1177	-0.0451
44	6	38	43	6	37	98263.0864	-0.043
45	6	40	44	6	39	98377.0619	-0.0115
45	5	40	44	5	39	98382.8428	0.0228
43	13	31	42	13	30	98397.6722	0.0571
43	13	30	42	13	29	98401.5707	0.0335
43	7	36	42	7	35	98721.7861	-0.04
43	12	32	42	12	31	98742.4451	0.0321
43	12	31	42	12	30	98782.1445	0.0082
47	4	44	46	4	43	98939.476	0.0003
47	3	44	46	3	43	98939.476	-0.0056
43	9	35	42	9	34	99032.0754	-0.0458
48	3	46	47	3	45	99261.8985	0.1142
48	2	46	47	2	45	99261.8985	0.1141
43	11	32	42	11	31	99446.8572	0.0429
42	8	34	41	8	33	99563.0777	-0.0271
49	1	48	48	1	47	99594.5019	0.0048
49	2	48	48	2	47	99594.5019	0.0048

42	9	33	41	9	32	99834.6979	0.0775
44	8	37	43	8	36	99882.9374	-0.0358
50	1	50	49	1	49	99931.6777	-0.023
50	0	50	49	0	49	99931.6777	-0.023
45	6	39	44	6	38	100202.608	-0.0733
46	5	41	45	5	40	100353.762	0.035
44	7	37	43	7	36	100521.353	-0.0234
47	5	43	46	5	42	100616.245	0.0828
47	4	43	46	4	42	100616.245	-0.0534
44	13	31	43	13	30	100786.779	0.0625
44	9	36	43	9	35	101197.51	-0.0844
49	2	47	48	2	46	101242.865	0.0227
49	3	47	48	3	46	101242.865	0.0228
43	8	35	42	8	34	101538.285	-0.1038
50	2	49	49	2	48	101575.835	0.0266
50	1	49	49	1	48	101575.835	0.0266
51	1	51	50	1	50	101913.004	-0.0216
51	0	51	50	0	50	101913.004	-0.0216
46	7	40	45	7	39	102109.624	-0.0196
47	6	42	46	6	41	102323.735	0.0187
43	9	34	42	9	33	102409.303	0.0239
48	5	44	47	5	43	102594.381	0.0398
48	5	44	47	5	43	102594.381	0.0398
48	4	44	47	4	43	102594.381	-0.0414

49	3	46	48	3	45		102899.853	-0.0667
45	13	32	44	13	31		103181.698	0.0321
50	3	48	49	3	47		103223.915	0.0369
50	2	48	49	2	47		103223.915	0.0369
51	1	50	50	1	49		103557.072	-0.0025
51	2	50	50	2	49		103557.072	-0.0025
46	8	39	45	8	38		103881.131	-0.0001
52	1	52	51	1	51		103894.3	0.0017
52	0	52	51	0	51		103894.3	0.0017
45	11	35	44	11	34		103963.542	0.01
47	6	41	46	6	40		104104.968	-0.0079
46	7	39	45	7	38		104207.481	-0.0635
48	6	43	47	6	42		104297.846	0.0097
48	5	43	47	5	42		104299.198	-0.0205
49	4	45	48	4	44		104572.775	-0.0122
49	5	45	48	5	44		104572.775	0.0361
51	2	49	50	2	48		105204.961	0.0733
51	3	49	50	3	48		105204.961	0.0733
52	2	51	51	2	50		105538.304	0.01
52	1	51	51	1	50		105538.304	0.01
46	13	34	45	13	33		105568.412	0.0853
46	13	33	45	13	32		105587.726	0.0472
47	8	40	46	8	39		105863.001	-0.081
53	0	53	52	0	52		105875.432	-0.0867

53	1	53	52	1	52		105875.432	-0.0867
48	6	42	47	6	41		106064.039	0.0603
47	7	40	46	7	39		106090.081	-0.1201
50	4	46	49	4	45		106551.366	0.0103
51	3	48	50	3	47		106860.554	0.0357
46	8	38	45	8	37		106958.083	-0.1038
52	2	50	51	2	49		107185.915	0.0472
52	3	50	51	3	49		107185.915	0.0472
54	0	54	53	0	53		107856.677	-0.0083
54	1	54	53	1	53		107856.677	-0.0083
48	7	41	47	7	40		107993.523	0.0201
49	7	43	48	7	42		108015.355	-0.0908
49	6	43	48	6	42		108026.434	-0.0871
50	5	45	49	5	44		108247.76	-0.3547
50	6	45	49	6	44		108247.76	0.1658
51	4	47	50	4	46		108530.112	0.0141
47	11	37	46	11	36		108742.349	-0.0568
52	3	49	51	3	48		108840.874	0.0189
53	3	51	52	3	50		109166.912	0.0961
53	2	51	52	2	50		109166.912	0.0961

S7.3 Measured frequencies and residuals (in MHz) for the rotational transitions of the vibrationally excited state $2\nu_{42}$ of CHT-1-CN-1 in the frequency range of 75-110 GHz using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	J'	K'_a	K'_c	Observed Freq. (MHz)	Residuals (MHz)
36	3	34	35	3	33	75357.9512	0.0667
37	1	36	36	1	35	75712.2828	-0.0477
37	2	36	36	2	35	75712.2828	-0.0467
38	0	38	37	0	37	76076.0093	-0.0309
36	3	33	35	3	32	77004.8206	0.0049
37	2	35	36	2	34	77337.1959	-0.0102
38	2	37	37	2	36	77692.3888	-0.0194
38	1	37	37	1	36	77692.3888	-0.0199
39	0	39	38	0	38	78056.243	-0.0182
36	5	32	35	5	31	78682.1363	-0.0154
38	2	36	37	2	35	79316.5793	0.0496
38	3	36	37	3	35	79316.5793	0.0714
39	2	38	38	2	37	79672.4517	-0.0125
39	1	38	38	1	37	79672.4517	-0.0128
40	0	40	39	0	39	80036.4667	0.0238
37	5	33	36	5	32	80656.1594	-0.0091

39	3	37	38	3	36	81295.9385	0.0458
39	2	37	38	2	36	81295.9385	0.0334
40	2	39	39	2	38	81652.5743	0.0797
40	1	39	39	1	38	81652.5743	0.0795
41	0	41	40	0	40	82016.591	0.0071
40	2	38	39	2	37	83275.322	0.0028
40	3	38	39	3	37	83275.322	0.0099
41	1	40	40	1	39	83632.4945	-0.0023
41	2	40	40	2	39	83632.4945	-0.0022
42	0	42	41	0	41	83996.6514	-0.0319
39	5	35	38	5	34	84603.8491	-0.0166
41	3	39	40	3	38	85254.7623	0.0057
41	2	39	40	2	38	85254.7623	0.0017
42	2	41	41	2	40	85612.4307	-0.0373
42	1	41	41	1	40	85612.4307	-0.0373
43	0	43	42	0	42	85976.711	-0.0287
40	5	36	39	5	35	86578.0502	0.04
40	5	36	39	5	35	86578.0502	0.04
40	4	36	39	4	35	86581.3793	-0.0726
41	4	38	40	4	37	86890.8297	0.0869
41	3	38	40	3	37	86890.8297	-0.0252
42	3	40	41	3	39	87234.2286	0.0106
42	2	40	41	2	39	87234.2286	0.0084
43	2	42	42	2	41	87592.3672	-0.0391

43	1	42	42	1	41	87592.3672	-0.0391
44	1	44	43	1	43	87956.8069	0.0548
40	6	35	39	6	34	88283.3572	-0.0498
41	5	37	40	5	36	88552.5102	0.0171
41	4	37	40	4	36	88554.5446	-0.0543
42	3	39	41	3	38	88868.7854	-0.0623
42	4	39	41	4	38	88868.7854	0.0032
43	2	41	42	2	40	89213.7351	0.0454
43	3	41	42	3	40	89213.7351	0.0466
44	2	43	43	2	42	89572.2639	-0.0455
44	1	43	43	1	42	89572.2639	-0.0455
45	0	45	44	0	44	89936.7361	0.0167
43	4	40	42	4	39	90847.0228	0.0664
44	2	42	43	2	41	91193.1853	0.0229
45	2	44	44	2	43	91552.1484	-0.0268
46	0	46	45	0	45	91916.6568	0.0163
42	6	37	41	6	36	92225.1799	-0.0135
45	3	43	44	3	42	93172.5638	-0.0675
45	2	43	44	2	42	93172.5638	-0.0679
46	2	45	45	2	44	93531.9739	-0.0281
46	1	45	45	1	44	93531.9739	-0.0281
47	0	47	46	0	46	93896.5213	0.0072
43	6	38	42	6	37	94195.6792	-0.0791
45	4	42	44	4	41	94803.6828	0.0507

45	3	42	44	3	41	94803.6828	0.0379
46	2	44	45	2	43	95152.054	-0.0385
46	3	44	45	3	43	95152.054	-0.0382
47	2	46	46	2	45	95511.7598	-0.0281
47	1	46	46	1	45	95511.7598	-0.0281
48	0	48	47	0	47	95876.3546	0.0153
43	6	37	42	6	36	96040.1681	0.0334
44	6	39	43	6	38	96166.5192	-0.0586
46	4	43	45	4	42	96782.1216	0.0218
47	2	45	46	2	44	97131.5274	-0.0122
47	3	45	46	3	44	97131.5274	-0.0121
48	1	47	47	1	46	97491.4896	-0.0416
48	2	47	47	2	46	97491.4896	-0.0416
49	0	49	48	0	48	97856.1449	0.0301
45	6	40	44	6	39	98137.8077	-0.017
48	2	46	47	2	45	99110.9852	0.0163
48	3	46	47	3	45	99110.9852	0.0164
49	2	48	48	2	47	99471.2621	0.0317
49	1	48	48	1	47	99471.2621	0.0317
47	4	43	46	4	42	100406.799	0.012
48	3	45	47	3	44	100739.31	0.0849
48	4	45	47	4	44	100739.31	0.0874
49	2	47	48	2	46	101090.358	-0.0184
49	3	47	48	3	46	101090.358	-0.0183

50	1	49	49	1	48	101450.89	0.0062
50	2	49	49	2	48	101450.89	0.0062
51	0	51	50	0	50	101815.543	0.0295
47	6	42	46	6	41	102081.849	-0.0278
48	4	44	47	4	43	102383.458	0.0296
49	3	46	48	3	45	102717.89	0.0347
49	4	46	48	4	45	102717.89	0.036
50	3	48	49	3	47	103069.73	-0.0275
50	2	48	49	2	47	103069.73	-0.0275
51	2	50	50	2	49	103430.507	0.0168
51	1	50	50	1	49	103430.507	0.0168
52	0	52	51	0	51	103795.205	0.0717
49	4	45	48	4	44	104360.336	0.0488
50	4	47	49	4	46	104696.573	0.0548
51	3	49	50	3	48	105049.087	-0.0236
51	2	49	50	2	48	105049.087	-0.0236
52	2	51	51	2	50	105409.95	-0.0969
53	0	53	52	0	52	105774.673	-0.0264
50	4	46	49	4	45	106337.398	0.0673
51	3	48	50	3	47	106675.178	-0.0277
51	4	48	50	4	47	106675.178	-0.0272
52	3	50	51	3	49	107028.421	-0.0102
52	2	50	51	2	49	107028.421	-0.0102
53	2	52	52	2	51	107389.627	0.0727

53	1	52	52	1	51		107389.627	0.0727
48	8	41	47	8	40		107530.083	0.05
49	7	43	48	7	42		107736.785	-0.0543
54	0	54	53	0	53		107754.243	0.0318
51	5	47	50	5	46		108314.48	-0.0397
52	4	49	51	4	48		108653.901	-0.0067
52	3	49	51	3	48		108653.901	-0.0069
53	2	51	52	2	50		109007.688	-0.0287
53	3	51	52	3	50		109007.688	-0.0287
54	2	53	53	2	52		109368.966	-0.0442
54	1	53	53	1	52		109368.966	-0.0442

S7.4 Measured frequencies and residuals (in MHz) for the rotational transitions of the vibrationally excited state $\nu_{42} + \nu_{41}$ of CHT-1-CN-1 in the frequency range of 75-110 GHz using SP-FIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	J'	K'_a	K'_c	Observed Freq. (MHz)	Residuals (MHz)
33	5	28	32	5	27	75116.4924	0.0441
36	3	34	35	3	33	75387.0013	0.0549
36	3	34	35	3	33	75387.011	0.0647
36	2	34	35	2	33	75387.011	-0.0143
38	1	38	37	1	37	76063.9975	0.0065
38	1	38	37	1	37	76063.9975	0.0065
38	1	37	37	1	36	77700.2398	0.0167
39	0	39	38	0	38	78043.643	-0.0127
39	1	39	38	1	38	78043.643	-0.0127
38	2	36	37	2	35	79344.366	-0.0609
38	3	36	37	3	35	79344.3705	-0.0302
38	2	36	37	2	35	79344.3705	-0.0564
40	0	40	39	0	39	80023.297	0.0144
40	1	40	39	1	39	80023.297	0.0144
38	4	35	37	4	34	81006.2552	0.0637
39	3	37	38	3	36	81323.198	-0.0102

40	1	39	39	1	38	81659.2216	0.0234
41	1	41	40	1	40	82002.875	0.0044
41	0	41	40	0	40	82002.875	0.0044
38	5	34	37	5	33	82699.9711	-0.0727
40	2	38	39	2	37	83302.064	0.0005
41	1	40	40	1	39	83638.6536	0.0054
42	0	42	41	0	41	83982.448	0.0294
42	1	42	41	1	41	83982.448	0.0294
38	6	33	37	6	32	84425.9149	0.0737
41	3	39	40	3	38	85280.9454	0.0143
41	2	39	40	2	38	85280.9454	0.0094
43	0	43	42	0	42	85961.9544	0.0291
43	1	43	42	1	42	85961.9544	0.0291
39	6	34	38	6	33	86401.1947	-0.0222
38	6	32	37	6	31	86814.892	0.0186
41	4	38	40	4	37	86937.4619	0.0666
41	4	38	40	4	37	86937.4619	0.0666
41	3	38	40	3	37	86937.4619	-0.0689
41	3	38	40	3	37	86937.4619	-0.0689
43	1	42	42	1	41	87597.458	-0.0026
44	0	44	43	0	43	87941.35	-0.0399
40	6	35	39	6	34	88373.7341	0.0015
42	4	39	41	4	38	88914.8317	0.0122
42	3	39	41	3	38	88914.8317	-0.0674

42	4	39	41	4	38		88914.8317	0.0122
44	1	43	43	1	42		89576.752	-0.0665
45	1	45	44	1	44		89920.8082	-0.0028
45	0	45	44	0	44		89920.8082	-0.0028
43	4	40	42	4	39		90892.3842	-0.0026
44	2	42	43	2	41		91217.637	-0.02
45	1	44	44	1	43		91556.154	0.0126
46	1	46	45	1	45		91900.1886	0.0008
46	0	46	45	0	45		91900.1886	0.0008
43	5	39	42	5	38		92569.1332	-0.0604
43	4	39	42	4	38		92570.1266	-0.0016
44	4	41	43	4	40		92870.0938	0.0164
44	3	41	43	3	40		92870.096	-0.0085
45	2	43	44	2	42		93196.576	0.0021
46	2	45	45	2	44		93535.426	-0.0016
46	1	45	45	1	44		93535.426	-0.0016
47	0	47	46	0	46		93879.514	-0.005
42	6	36	41	6	35		94252.9925	-0.1114
45	3	42	44	3	41		94847.8762	-0.0125
45	4	42	44	4	41		94847.8762	0.0033
46	3	44	45	3	43		95175.426	-0.0596
47	1	46	46	1	45		95514.6659	-0.0093
47	1	46	46	1	45		95514.673	-0.0021
48	1	48	47	1	47		95858.818	0.0144

48	1	48	47	1	47	95858.8203	0.0167
48	0	48	47	0	47	95858.8203	0.0167
46	4	43	45	4	42	96825.7991	0.0421
46	3	43	45	3	42	96825.7991	0.0329
48	1	47	47	1	46	97493.7951	-0.0873
48	2	47	47	2	46	97493.82	-0.0624
49	0	49	48	0	48	97838.0685	0.0279
49	1	49	48	1	48	97838.0685	0.0279
47	4	44	46	4	43	98803.7284	0.0136
47	3	44	46	3	43	98803.729	0.0089
49	1	48	48	1	47	99473.0408	-0.0069
49	1	48	48	1	47	99473.05	0.0023
49	2	48	48	2	47	99473.05	0.0023
50	0	50	49	0	49	99817.2692	0.0403
50	1	50	49	1	49	99817.2692	0.0403
46	6	41	45	6	40	100196.191	-0.0439
48	3	45	47	3	44	100781.711	-0.0252
48	4	45	47	4	44	100781.753	0.02
49	2	47	48	2	46	101112.149	0.0053
50	1	49	49	1	48	101452.2	0.0307
47	6	42	46	6	41	102167.828	0.0882
48	5	44	47	5	43	102446.66	0.0207
48	4	44	47	4	43	102446.66	-0.0517
49	3	46	48	3	45	102759.784	-0.0181

50	2	48	49	2	47		103090.974	-0.0161
51	2	50	50	2	49		103431.218	-0.0287
51	1	50	50	1	49		103431.25	0.0031
49	5	45	48	5	44		104422.892	0.0026
50	4	47	49	4	46		104737.935	0.0295
50	3	47	49	3	46		104737.937	0.0301
51	2	49	50	2	48		105069.784	-0.0266
53	0	53	52	0	52		105754.495	0.0038
53	1	53	52	1	52		105754.495	0.0038
50	4	46	49	4	45		106399.364	0.0121
51	4	48	50	4	47		106716.08	0.0397
51	3	48	50	3	47		106716.104	0.0632
54	0	54	53	0	53		107733.505	0.0309
51	4	47	50	4	46		108376.001	0.0613
52	4	49	51	4	48		108694.172	-0.0235
53	2	51	52	2	50		109027.321	-0.041
54	2	53	53	2	52		109368.146	-0.048
54	1	53	53	1	52		109368.199	0.0046

S7.5 Measured frequencies and residuals (in MHz) for the rotational transitions of the vibrationally excited state $2\nu_{38}$ of CHT-1-CN-1 in the frequency range of 75-110 GHz using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	J'	K'_a	K'_c	Observed Freq. (MHz)	Residuals (MHz)
37	1	36	36	1	35	75695.1736	-0.0132
37	2	36	36	2	35	75695.1736	-0.0123
38	1	38	37	1	37	76065.6625	-0.0163
38	0	38	37	0	37	76065.6625	-0.0163
37	2	35	36	2	34	77312.9624	-0.0569
38	1	37	37	1	36	77675.0574	-0.0185
38	2	37	37	2	36	77675.0574	-0.018
39	1	39	38	1	38	78045.7305	0.0189
39	0	39	38	0	38	78045.7305	0.0189
39	1	38	38	1	37	79654.9576	0.0158
39	2	38	38	2	37	79654.9576	0.016
40	1	40	39	1	39	80025.7098	0.0053
40	0	40	39	0	39	80025.7098	0.0053
40	1	39	39	1	38	81634.7813	-0.0003
40	1	39	39	1	38	81634.7813	-0.0003

41	1	41	40	1	40	82005.6415	-0.015
41	0	41	40	0	40	82005.6415	-0.015
40	2	38	39	2	37	83250.598	0.026
41	2	40	40	2	39	83614.5592	-0.033
41	1	40	40	1	39	83614.5592	-0.0331
42	1	42	41	1	41	83985.5571	-0.0089
42	0	42	41	0	41	83985.5571	-0.0089
41	2	39	40	2	38	85229.8366	0.0127
41	3	39	40	3	38	85229.8366	0.0166
42	2	41	41	2	40	85594.3759	0.0042
42	1	41	41	1	40	85594.3759	0.0041
43	1	43	42	1	42	85965.485	0.0527
43	0	43	42	0	42	85965.485	0.0527
41	4	38	40	4	37	86858.6466	-0.0053
42	3	40	41	3	39	87209.1136	0.023
42	2	40	41	2	39	87209.1136	0.0209
43	2	42	42	2	41	87574.1518	0.0344
43	1	42	42	1	41	87574.1518	0.0344
44	0	44	43	0	43	87945.2748	0.0209
44	1	44	43	1	43	87945.2748	0.0209
42	4	39	41	4	38	88836.4729	-0.0368
42	4	39	41	4	38	88836.4729	-0.0368
43	3	41	42	3	40	89188.3809	0.0117
43	2	41	42	2	40	89188.3809	0.0105

45	1	45	44	1	44	89925.0282	-0.0017
45	0	45	44	0	44	89925.0282	-0.0017
44	3	42	43	3	41	91167.6653	0.016
44	2	42	43	2	41	91167.6653	0.0153
45	1	44	44	1	43	91533.4859	-0.0133
45	2	44	44	2	43	91533.4859	-0.0132
46	0	46	45	0	45	91904.7793	0.0203
46	1	46	45	1	45	91904.7793	0.0203
44	4	41	43	4	40	92792.5633	-0.0399
45	2	43	44	2	42	93146.9167	-0.0085
45	3	43	44	3	42	93146.9167	-0.0081
46	1	45	45	1	44	93513.1137	-0.0176
46	2	45	45	2	44	93513.1137	-0.0176
47	1	47	46	1	46	93884.3991	-0.0412
47	0	47	46	0	46	93884.3991	-0.0412
45	3	42	44	3	41	94770.7559	-0.058
46	3	44	45	3	43	95126.1974	0.0068
47	2	46	46	2	45	95492.6895	-0.0324
47	1	46	46	1	45	95492.6895	-0.0324
48	1	48	47	1	47	95864.0839	0.0115
48	0	48	47	0	47	95864.0839	0.0115
46	3	43	45	3	42	96749.1604	0.074
47	3	45	46	3	44	97105.4494	0.0076
47	2	45	46	2	44	97105.4494	0.0075

48	2	47	47	2	46	97472.2273	-0.0419
48	1	47	47	1	46	97472.2273	-0.0419
49	0	49	48	0	48	97843.6917	0.0372
49	1	49	48	1	48	97843.6917	0.0372
47	4	44	46	4	43	98727.4281	0.0059
47	4	44	46	4	43	98727.4281	0.0059
49	2	48	48	2	47	99451.7498	-0.0218
49	1	48	48	1	47	99451.7498	-0.0218
50	1	50	49	1	49	99823.1712	-0.014
50	0	50	49	0	49	99823.1712	-0.014
48	4	45	47	4	44	100705.888	0.0703
49	3	47	48	3	46	101063.886	0.0026
49	2	47	48	2	46	101063.886	0.0025
51	1	51	50	1	50	101802.708	0.0441
51	0	51	50	0	50	101802.708	0.0441
49	4	46	48	4	45	102684.322	0.0679
50	3	48	49	3	47	103043.06	-0.0054
50	2	48	49	2	47	103043.06	-0.0055
52	0	52	51	0	51	103782.099	0.0108
51	2	49	50	2	48	105022.217	-0.0016
51	3	49	50	3	48	105022.217	-0.0016
53	0	53	52	0	52	105761.418	-0.0406
53	1	53	52	1	52	105761.418	-0.0406
52	3	50	51	3	49	107001.325	-0.0131

52	2	50	51	2	49		107001.325	-0.0131
53	2	52	52	2	51		107369.311	0.0101
53	1	52	52	1	51		107369.311	0.0101
54	0	54	53	0	53		107740.776	0.0026
54	1	54	53	1	53		107740.776	0.0026
53	3	51	52	3	50		108980.427	0.006
53	2	51	52	2	50		108980.427	0.006
54	1	53	53	1	52		109348.536	-0.0204
54	2	53	53	2	52		109348.536	-0.0204

S7.6 Measured frequencies and residuals (in MHz) for the rotational transitions of the vibrationally excited state $2\nu_{40}$ of CHT-1-CN-1 in the frequency range of 75-110 GHz using SPFIT/SPCAT suite of programs from Pickett.

J	K_a	K_c	J'	K'_a	K'_c	Observed Freq. (MHz)	Residuals (MHz)
37	2	36	36	2	35	75714.9051	-0.06
37	1	36	36	1	35	75714.9051	-0.0612
38	1	38	37	1	37	76058.3251	-0.0266
38	0	38	37	0	37	76058.3251	-0.0267
37	2	35	36	2	34	77359.8604	0.1321
37	3	35	36	3	34	77359.8604	0.1788
38	1	37	37	1	36	77694.2943	-0.0735
38	2	37	37	2	36	77694.2943	-0.0728
39	1	39	38	1	38	78037.8685	-0.0172
39	0	39	38	0	38	78037.8685	-0.0172
38	3	36	37	3	35	79338.3383	0.0053
38	2	36	37	2	35	79338.3383	-0.0216
39	2	38	38	2	37	79673.6915	-0.0585
40	1	40	39	1	39	80017.3619	-0.0207
40	0	40	39	0	39	80017.3619	-0.0207
39	2	37	38	2	36	81317.0504	-0.001

39	3	37	38	3	36	81317.0504	0.0144
40	2	39	39	2	38	81653.0467	-0.064
41	1	41	40	1	40	81996.891	0.0495
41	0	41	40	0	40	81996.891	0.0495
40	3	38	39	3	37	83295.7155	-0.0644
41	1	40	40	1	39	83632.4945	0.0477
41	2	40	40	2	39	83632.4945	0.0478
41	3	39	40	3	38	85274.5024	-0.0528
41	2	39	40	2	38	85274.5024	-0.0578
42	1	41	41	1	40	85611.8575	0.1021
42	2	41	41	2	40	85611.8575	0.1021
42	2	40	41	2	39	87253.3597	0.0036
42	3	40	41	3	39	87253.3597	0.0065
42	3	39	41	3	38	88908.232	-0.0533
43	2	41	42	2	40	89232.2333	0.0653
43	3	41	42	3	40	89232.2333	0.0669
43	3	40	42	3	39	90885.7282	-0.0039
46	1	46	45	1	45	91893.5988	0.0735
46	0	46	45	0	45	91893.5988	0.0735
44	3	41	43	3	40	92863.3308	0.0122
47	0	47	46	0	46	93872.7502	0.0177
47	1	47	46	1	46	93872.7502	0.0177
48	1	48	47	1	47	95851.9017	0.0077
48	0	48	47	0	47	95851.9017	0.0077

49	1	49	48	1	48	97831.0036	-0.0052
49	0	49	48	0	48	97831.0036	-0.0052
49	2	48	48	2	47	99465.9982	0.0197
49	1	48	48	1	47	99465.9982	0.0197
50	1	49	49	1	48	101444.947	-0.0511
51	0	51	50	0	50	101789.178	0.0838
51	1	51	50	1	50	101789.178	0.0838
51	1	50	50	1	49	103423.974	0
52	0	52	51	0	51	103768.04	-0.022
52	1	52	51	1	51	103768.04	-0.022
51	3	49	50	3	48	105062.609	0.0872
51	2	49	50	2	48	105062.609	0.0872
52	1	51	51	1	50	105402.852	-0.0525
53	0	53	52	0	52	105746.958	-0.0223
53	1	53	52	1	52	105746.958	-0.0223
53	0	53	52	0	52	105746.958	-0.0223
52	2	50	51	2	49	107041.228	-0.0048
52	3	50	51	3	49	107041.228	-0.0048
53	1	52	52	1	51	107381.736	-0.0528
54	1	54	53	1	53	107725.837	-0.0087
54	0	54	53	0	53	107725.837	-0.0087
54	2	53	53	2	52	109360.632	0.0065
54	1	53	53	1	52	109360.632	0.0065

References

- D. Schmitz, V. A. Shubert, T. Betz and M. Schnell, *Journal of Molecular Spectroscopy*, 2012, **280**, 77–84.
- C. Pérez, A. Krin, A. L. Steber, J. C. López, Z. Kisiel and M. Schnell, *The Journal of Physical Chemistry Letters*, 2016, **7**, 154–160.
- M. Fatima, C. Pérez, B. E. Arenas, M. Schnell and A. L. Steber, *Physical Chemistry Chemical Physics*, 2020, **22**, 17042–17051.
- J. L. Neill, B. J. Harris, A. L. Steber, K. O. Douglass, D. F. Plusquellic and B. H. Pate, *Optics Express*, 2013, **21**, 19743.
- B. E. Arenas, S. Gruet, A. L. Steber, B. M. Giuliano and M. Schnell, *Physical Chemistry Chemical Physics*, 2017, **19**, 1751–1756.