

Supplementary material:
Electron-withdrawing effects on the molecular structure of
2- and 3-nitrobenzonitrile revealed by broadband rotational
spectroscopy and their comparison with 4-nitrobenzonitrile

Jack B. Graneek¹, William C. Bailey², and Melanie Schnell^{3,*}

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^{1,3}*Deutsches Elektronen-Synchrotron, Notkestraße 85, D-22607 Hamburg, Germany*
CAU Kiel, Institute of Physical Chemistry, Max-Eyth-Straße 1, D-24118 Kiel, Germany
Max-Planck-Institut für Struktur und Dynamik der Materie
Luruper Chaussee 149, D-22761 Hamburg, Germany

²*Chemistry-Physics Department, Kean University, 1000 Morris Avenue, Union, NJ, USA*

Rotational spectroscopy parameters determined via a B3LYP/aug-cc-pVTZ (GD3BJ) calculation for each NBN molecule, the rotational constants determined for each isotopologue of 2- and 3-NBN, experimentally determined and calculated bond lengths/angles of 2- and 3-NBN, as well as the calculated bond lengths/angles of 4-NBN. Lists of all the fitted transitions for each isotopologue of 2- and 3-NBN are also provided.

[*] melanie.schnell@desy.de

Table S1: Spectroscopic constants of 2-, 3-, 4-nitrobenzonitrile (NBN) determined experimentally and via quantum-chemical calculations including and excluding Grimme’s empirical dispersion. N₁₁ refers to the nitrogen atom of the nitro group and N₁₅ to the nitrogen atom of the nitrile group. The standard errors of the obtained values are included in parentheses, and values for the number of lines assigned (N_{lines}) and the root-mean-square deviation of the fit (σ) are also provided.

Parameter	Experiment		B3LYP/aug-cc-pVTZ			B3LYP(GD3BJ)/aug-cc-pVTZ		
	2-NBN	3-NBN	2-NBN	3-NBN	4-NBN	2-NBN	3-NBN	4-NBN
A [MHz]	1506.5484(2)	2269.92862(9)	1499.04	2282.75	3985.67	1504.33	2285.42	3986.58
B [MHz]	1240.8070(2)	749.97847(4)	1254.69	751.43	593.84	1256.42	752.90	595.16
C [MHz]	685.2525(2)	563.99011(3)	683.01	565.33	516.84	684.62	566.33	517.85
D _K [kHz]	0.149(5)
D _{JK} [kHz]	-0.267(6)
D _J [kHz]	0.162(6)
χ_{aa} (N ₁₁) [MHz]	-0.779(1)	-0.727(2)	-0.9335	-0.8777	-1.1533	-0.9390	-0.8832	-1.1619
χ_{bb-cc} (N ₁₁) [MHz]	-0.470(3)	-0.766(3)	-1.0777	-1.2983	-1.0238	-1.0794	-1.3006	-1.0233
χ_{aa} (N ₁₅) [MHz]	-0.401(1)	-2.518(1)	-0.2163	-2.8007	-4.8451	-0.2691	-2.8040	-4.8479
χ_{bb-cc} (N ₁₅) [MHz]	-4.197(2)	-1.528(2)	-5.2325	-1.7141	0.1309	-5.2073	-1.7158	0.1286
$\mu_a/\mu_b/\mu_c$ [D]	6.69/1.94/0	0.14/4.38/0	0.09/0/0	6.70/1.90/0	0.14/4.38/0	0.09/0/0
N _{lines}	289	256
σ [kHz]	4.9	3.2

Table S2: Comparison of the nuclear quadrupole coupling constants (NQCCs) determined experimentally to those obtained via the quantum-chemical calculations described in Section 3.

Parameter	2-NBN			3-NBN			4-NBN	
	Exp.	B3LYP	B3PW91	Exp.	B3LYP	B3PW91	B3LYP	B3PW91
χ_{aa} (N ₁₁) [MHz]	-0.779(1)	-0.9335	-0.805	-0.727(2)	-0.8777	-0.743	-1.1533	-1.050
$\chi_{bb} - \chi_{cc}$ (N ₁₁) [MHz]	-0.470(3)	-1.0777	-0.525	-0.766(3)	-1.2983	-0.749	-1.0238	-0.447
χ_{ab} (N ₁₁) [MHz]	...	-0.2907	-0.357	...	-0.4956	-0.553	0	0
χ_{aa} (N ₁₅) [MHz]	-0.401(1)	-0.2163	-0.367	-2.518(1)	-2.8007	-2.548	-4.8451	-4.369
$\chi_{bb} - \chi_{cc}$ (N ₁₅) [MHz]	-4.197(2)	-5.2325	-4.607	-1.528(2)	-1.7141	-1.528	0.1309	0.111
χ_{ab} (N ₁₅) [MHz]	...	3.2362	2.957	...	3.2931	2.957	0	0

Table S3: NQCCs of 2- and 3-NBN in principal axes of the quadrupolar system. The experimentally determined NQCCs utilised the B3PW91 χ_{ab} values provided in Table S2 to complete the nuclear quadrupole tensor for the respective nitrogen nuclei. A comparison to the NQCCs obtained via the quantum-chemical calculations described in Section 3 is also provided.

Parameter	2-NBN		3-NBN	
	Exp.	B3PW91	Exp.	B3PW91
χ_{xx} (N ₁₁) [MHz]	0.275(3)	0.259	0.283(2)	0.292
χ_{yy} (N ₁₁) [MHz]	0.625(3)	0.665	0.747(3)	0.746
χ_{zz} (N ₁₁) [MHz]	-0.900(1)	-0.924	-1.030(2)	-1.038
χ_{xx} (N ₁₅) [MHz]	1.901(1)	1.841	2.307(2)	2.310
χ_{yy} (N ₁₅) [MHz]	2.229(2)	2.487	2.023(2)	2.038
χ_{zz} (N ₁₅) [MHz]	-4.200(1)	-4.328	-4.330(1)	4.348

Table S4: Rotational constants determined from the assignment for each isotopologue of 2-NBN. Also included are values for the number of lines assigned (N_{lines}) and the root-mean-square deviation of the fits (σ), which are needed for the subsequent Kraitchman calculations used to determine the substituted structure (r_s). Centrifugal distortion constants in square brackets have been fixed to the values of the parent isotopologue.

Parameter	Parent	C ₁	C ₂	C ₃	C ₄	C ₅
A [MHz]	1506.5484(2)	1505.4259(3)	1497.0687(9)	1502.0293(9)	1506.128(1)	1499.772(1)
B [MHz]	1240.8070(2)	1240.8096(3)	1237.3855(9)	1223.6338(6)	1219.4415(3)	1232.465(1)
C [MHz]	685.2525(2)	685.0559(2)	682.2407(4)	679.0553(4)	678.5962(2)	681.3042(5)
D _K [kHz]	0.149(5)	[0.149]	0.28(5)	0.14(3)	[0.149]	0.28(5)
D _{JK} [kHz]	-0.267(6)	[-0.267]	-0.44(8)	-0.35(5)	[-0.267]	-0.57(8)
D _J [kHz]	0.162(6)	[0.162]	0.19(4)	0.21(2)	[0.162]	0.26(5)
χ_{aa} (N ₁₁) [MHz]	-0.779(1)	-0.79(1)	-0.77(2)	-0.79(2)	-0.77(2)	-0.78(2)
χ_{bb} (N ₁₁) [MHz]	0.155(3)	0.17(1)	0.15(2)	0.18(2)	0.14(2)	0.19(2)
χ_{cc} (N ₁₁) [MHz]	0.624(3)	0.618(6)	0.622(8)	0.611(6)	0.629(6)	0.58(1)
χ_{aa} (N ₁₅) [MHz]	-0.401(1)	-0.40(1)	-0.54(3)	-0.59(2)	-0.34(1)	-0.39(3)
χ_{bb} (N ₁₅) [MHz]	-1.898(2)	-1.91(2)	-1.75(3)	-1.72(2)	-1.96(1)	-1.98(3)
χ_{cc} (N ₁₅) [MHz]	2.299(2)	2.305(6)	2.290(7)	2.310(5)	2.300(5)	2.32(1)
N _{lines}	289	82	68	101	77	68
σ [kHz]	4.9	6.3	6.1	6.8	5.9	7.5
Parameter	C ₆	N ₁₁	O ₁₂	O ₁₃	C ₁₄	N ₁₅

A [MHz]	1503.4160(8)	1502.0832(7)	1505.460(3)(2)	1466.823(2)	1490.976(1)	1473.1843(5)
B [MHz]	1240.552(1)	1235.2374(7)	1210.8157(9)	1224.6782(4)	1239.2828(5)	1234.3873(3)
C [MHz]	684.5270(4)	682.6445(3)	676.1177(6)	672.2623(2)	681.5582(2)	676.3515(2)
D_K [kHz]	0.30(5)	0.30(5)	0.74(5)	[0.149]	[0.149]	[0.149]
D_{JK} [kHz]	-0.54(8)	-0.42(8)	-0.10(7)	[-0.267]	[-0.267]	[-0.267]
D_J [kHz]	0.27(5)	0.18(4)	0.37(3)	[0.162]	[0.162]	[0.162]
χ_{aa} (N_{11}) [MHz]	-0.78(2)	...	-0.79(1)	-0.79(2)	-0.75(2)	-0.73(1)
χ_{bb} (N_{11}) [MHz]	0.17(2)	...	0.17(1)	0.19(2)	0.13(2)	0.12(1)
χ_{cc} (N_{11}) [MHz]	0.616(7)	...	0.621(7)	0.60(1)	0.616(7)	0.616(4)
χ_{aa} (N_{15}) [MHz]	-0.39(2)	-0.295(7)	-0.35(1)	-0.19(2)	-0.51(2)	...
χ_{bb} (N_{15}) [MHz]	-1.92(2)	-2.007(7)	-1.95(1)	-2.25(2)	-1.80(2)	...
χ_{cc} (N_{15}) [MHz]	2.306(5)	2.301(3)	2.300(6)	2.45(1)	2.302(6)	...
N_{lines}	63	51	42	37	61	43
σ [kHz]	5.7	3.8	3.3	4.4	6.5	4.7

Table S5: Rotational constants determined from the assignment for each isotopologue of 3-NBN. Also included are values for the number of lines assigned (N_{lines}) and the root-mean-square deviation of the fits (σ), which are needed for the subsequent Kraitchman calculations used to determine the substituted structure (r_s).

Parameter	Parent	C ₁	C ₂	C ₃	C ₄	C ₅
A [MHz]	2269.92862(9)	2269.8100(5)	2246.7476(4)	2223.0867(4)	2249.3747(3)	2269.9558(3)
B [MHz]	749.97847(4)	749.2439(2)	749.2355(2)	749.7859(3)	747.1401(2)	747.3525(2)
C [MHz]	563.99011(3)	563.5674(2)	562.1295(2)	560.9442(2)	561.1126(2)	562.5056(2)
χ_{aa} (N_{11}) [MHz]	-0.727(2)	-0.720(9)	-0.718(9)	-0.679(9)	-0.73(1)	-0.718(7)
χ_{bb} (N_{11}) [MHz]	-0.020(3)	-0.03(1)	-0.03(1)	-0.06(1)	-0.02(1)	-0.025(8)
χ_{cc} (N_{11}) [MHz]	0.747(3)	0.75(1)	0.74(1)	0.73(1)	0.75(1)	0.743(8)
χ_{aa} (N_{15}) [MHz]	-2.518(1)	-2.521(8)	-2.521(7)	-2.498(6)	-2.483(6)	-2.506(5)
χ_{bb} (N_{15}) [MHz]	0.495(2)	0.513(9)	0.510(8)	0.483(8)	0.470(7)	0.491(6)

χ_{cc} (N_{15}) [MHz]	2.023(2)	2.009(9)	2.011(8)	2.016(8)	2.014(7)	2.015(6)
N_{lines}	262	67	99	93	86	87
σ [kHz]	3.2	6.4	7.6	7.3	6.2	5.6
Parameter	C_6	N_{11}	O_{12}	O_{13}	C_{14}	N_{15}
A [MHz]	2265.7923(3)	2266.8347(3)	2208.6543(6)	2269.5166(6)	2264.7342(3)	2252.9016(3)
B [MHz]	749.8961(2)	744.9908(2)	740.0299(2)	728.8255(3)	741.5529(2)	734.6684(2)
C [MHz]	563.6895(2)	560.9750(2)	554.5656(2)	551.9265(2)	558.8962(2)	554.2600(1)
χ_{aa} (N_{11}) [MHz]	-0.723(8)	...	-0.80(2)	-0.70(1)	-0.721(8)	-0.717(6)
χ_{bb} (N_{11}) [MHz]	-0.03(1)	...	-0.05(1)	-0.03(2)	-0.023(9)	-0.024(7)
χ_{cc} (N_{11}) [MHz]	0.76(1)	...	0.76(1)	0.73(2)	0.744(9)	0.741(7)
χ_{aa} (N_{15}) [MHz]	-2.521(5)	-2.496(8)	-2.40(2)	-2.51(1)	-2.541(5)	...
χ_{bb} (N_{15}) [MHz]	0.505(7)	0.449(8)	0.41(1)	0.51(1)	0.521(6)	...
χ_{cc} (N_{15}) [MHz]	2.016(7)	2.048(8)	1.99(1)	2.01(1)	2.021(6)	...
N_{lines}	90	63	43	45	106	51
σ [kHz]	6.2	5.5	5.8	6.5	6.2	4.5

Table S6: Experimentally determined and calculated bond lengths of 2-NBN; r_s -structure (Kraitchman’s planar equations), $r_m^{(1)}$ -structure (mass-dependent least-square fit), r_e -structures (B3LYP/aug-cc-pVTZ including and excluding GD3BJ).

Bond lengths	Planar r_s (Å)	$r_m^{(1)}$ (Å)	B3LYP r_e (Å)	B3LYP(GD3BJ) r_e (Å)
C ₁ –C ₂	...	1.386(4)	1.386	1.385
C ₂ –C ₃	1.398(2)	1.387(5)	1.387	1.386
C ₃ –C ₄	1.397(5)	1.390(8)	1.390	1.390
C ₄ –C ₅	1.391(3)	1.386(5)	1.386	1.385
C ₅ –C ₆	1.419(5)	1.401(3)	1.401	1.400
C ₆ –C ₁	...	1.402(1)	1.402	1.401
C ₁ –N ₁₁	...	1.471(3)	1.479	1.477
N ₁₁ –O ₁₂	1.110(2)	1.205(7)	1.218	1.218
N ₁₁ –O ₁₃	1.220(2)	1.203(7)	1.221	1.221
O ₁₂ ···O ₁₃	1.985(4)	2.137(9)	2.166	2.166
C ₆ –C ₁₄	1.431(4)	1.439(4)	1.430	1.429
C ₁₄ –N ₁₅	1.159(2)	1.152(6)	1.152	1.151

Table S7: Experimentally determined and calculated bond angles of 2-NBN; r_s -structure (Kraitchman’s planar equations), $r_m^{(1)}$ -structure (mass-dependent least-square fit), r_e -structure (B3LYP/aug-cc-pVTZ including and excluding GD3BJ).

Bond angles	Planar r_s (°)	$r_m^{(1)}$ (°)	B3LYP r_e (°)	B3LYP(GD3BJ) r_e (°)
∠C ₁ C ₂ C ₃	...	119.8(2)	119.78	119.72
∠C ₂ C ₃ C ₄	120.1(1)	119.9(3)	119.91	119.93
∠C ₃ C ₄ C ₅	120.1(1)	120.2(3)	120.18	120.20
∠C ₄ C ₅ C ₆	120.5(2)	120.9(3)	120.93	120.84
∠C ₅ C ₆ C ₁	...	117.8(2)	117.83	117.91
∠C ₆ C ₁ C ₂	...	121.4(2)	121.37	121.41
∠C ₂ C ₁ N ₁₁	...	117.5(2)	117.52	117.60
∠C ₁ N ₁₁ O ₁₂	...	117.5(2)	117.54	117.51
∠C ₁ N ₁₁ O ₁₃	...	117.3(4)	117.34	117.33
∠O ₁₂ N ₁₁ O ₁₃	116.8(2)	125.1(5)	125.12	125.15
∠C ₅ C ₆ C ₁₄	116.1(2)	116.6(2)	116.66	116.71
∠C ₆ C ₁₄ N ₁₅	173.4(2)	171.7(5)	171.70	171.65

Table S8: Experimentally determined and calculated bond lengths of 3-NBN; r_s -structure (Kraitchman’s planar equations), $r_m^{(1)}$ -structure (mass-dependent least-square fit), r_e -structure (B3LYP/aug-cc-pVTZ including and excluding GD3BJ).

Bond lengths	Planar r_s (Å)	$r_m^{(1)}$ (Å)	B3LYP r_e (Å)	B3LYP(GD3BJ) r_e (Å)
C ₁ –C ₂	1.41(1)	1.387(3)	1.387	1.386
C ₂ –C ₃	1.393(4)	1.389(3)	1.389	1.388
C ₃ –C ₄	1.395(3)	1.387(3)	1.387	1.387
C ₄ –C ₅	...	1.400(2)	1.400	1.399
C ₅ –C ₆	...	1.396(1)	1.396	1.395
C ₆ –C ₁	1.318(9)	1.384(2)	1.384	1.383
C ₁ –N ₁₁	1.477(7)	1.483(4)	1.480	1.478
N ₁₁ –O ₁₂	1.228(3)	1.232(5)	1.220	1.220
N ₁₁ –O ₁₃	1.231(6)	1.230(6)	1.221	1.221
O ₁₂ ...O ₁₃	2.183(9)	2.185(6)	2.166	2.167
C ₅ –C ₁₄	...	1.431(2)	1.431	1.429
C ₁₄ –N ₁₅	1.157(1)	1.152(3)	1.152	1.151

Table S9: Experimentally determined and calculated bond angles of 3-NBN; r_s -structure (Kraitchman’s planar equations), $r_m^{(1)}$ -structure (mass-dependent least-square fit), r_e -structure (B3LYP/aug-cc-pVTZ including and excluding GD3BJ).

Bond angles	Planar r_s (°)	$r_m^{(1)}$ (°)	B3LYP r_e (°)	B3LYP(GD3BJ) r_e (°)
\angle C ₁ C ₂ C ₃	117.7(2)	118.6(2)	118.66	118.66
\angle C ₂ C ₃ C ₄	120.3(1)	120.4(1)	120.38	120.36
\angle C ₃ C ₄ C ₅	...	120.1(2)	120.06	120.03
\angle C ₄ C ₅ C ₆	...	120.1(1)	120.14	120.21
\angle C ₅ C ₆ C ₁	...	118.4(1)	118.35	118.27
\angle C ₆ C ₁ C ₂	124.6(5)	122.4(1)	122.42	122.47
\angle C ₂ C ₁ N ₁₁	116.6(5)	119.0(2)	118.96	118.94
\angle C ₁ N ₁₁ O ₁₂	116.4(5)	117.5(4)	117.50	117.47
\angle C ₁ N ₁₁ O ₁₃	118.5(7)	117.4(3)	117.36	117.36
\angle O ₁₂ N ₁₁ O ₁₃	125.4(4)	125.1(5)	125.14	125.17
\angle C ₄ C ₅ C ₁₄	...	120.0(1)	119.97	119.93
\angle C ₅ C ₁₄ N ₁₅	...	179.6(3)	179.57	179.57

Table S10: Calculated r_e bond lengths and angles of 4-NBN using the aug-cc-pVTZ basis set with the B3LYP hybrid functional including and excluding Grimme’s empirical dispersion (GD3BJ).

Bond lengths	B3LYP r_e (Å)	B3LYP(GD3BJ) r_e (Å)	Bond angles	B3LYP r_e (°)	B3LYP(GD3BJ) r_e (°)
C ₁ –C ₂	1.385	1.383	∠C ₁ C ₂ C ₃	119.91	119.85
C ₂ –C ₃	1.399	1.399	∠C ₂ C ₃ C ₄	120.30	120.40
C ₃ –C ₄	1.399	1.399	∠C ₃ C ₄ C ₅	119.91	119.85
C ₄ –C ₅	1.385	1.383	∠C ₄ C ₅ C ₆	118.78	118.74
C ₅ –C ₆	1.387	1.386	∠C ₅ C ₆ C ₁	122.32	122.41
C ₆ –C ₁	1.387	1.386	∠C ₆ C ₁ C ₂	118.78	118.74
C ₆ –N ₁₁	1.478	1.478	∠C ₅ C ₆ N ₁₁	118.84	118.80
N ₁₁ –O ₁₂	1.221	1.221	∠C ₆ N ₁₁ O ₁₂	117.45	117.44
N ₁₁ –O ₁₃	1.221	1.221	∠C ₆ N ₁₁ O ₁₃	117.45	117.44
O ₁₂ ⋯O ₁₃	2.167	2.167	∠O ₁₂ N ₁₁ O ₁₃	125.09	125.12
C ₃ –C ₁₄	1.430	1.429	∠C ₄ C ₃ C ₁₄	119.85	119.80
C ₁₄ –N ₁₅	1.152	1.152	∠C ₃ C ₁₄ N ₁₅	180.00	180.00

Table S11: List of lines assigned for the parent isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2191.328	2191.3293	-0.0013	1	1	1	2	2	0	0	0	2	2
2192.7515	2192.7511	0.0004	1	1	1	1	1	0	0	0	2	2
2256.1355	2256.1328	0.0027	5	4	1	2	6	5	3	2	2	6
2256.3866	2256.3907	-0.0041	5	4	1	1	6	5	3	2	1	6
2274.2639	2274.2596	0.0043	5	3	2	1	5	5	3	3	1	5
2274.3945	2274.3902	0.0043	5	3	2	2	7	5	3	3	2	7
2275.0317	2275.0301	0.0016	5	3	2	2	6	5	3	3	2	6
2463.1512	2463.156	-0.0048	2	2	1	1	2	2	1	2	2	2
2463.3907	2463.3921	-0.0014	2	2	1	2	2	2	1	2	1	2
2463.5979	2463.5919	0.006	2	2	1	2	4	2	1	2	2	4
2462.9846	2462.9855	-0.0009	2	2	1	2	1	2	1	2	2	0
2463.0775	2463.0754	0.0021	2	2	1	2	0	2	1	2	2	1
2463.8686	2463.868	0.0006	2	2	1	1	3	2	1	2	1	3
2464.0387	2464.0385	0.0002	2	2	1	2	3	2	1	2	1	3
2464.4691	2464.4643	0.0048	2	2	1	1	3	2	1	2	2	3
2464.8139	2464.814	-0.0001	2	2	1	0	2	2	1	2	0	2
2537.9435	2537.9469	-0.0034	2	2	1	2	1	2	0	2	2	0
2538.2894	2538.2896	-0.0002	2	2	1	2	2	2	0	2	1	2
2538.5048	2538.5078	-0.003	2	2	1	2	4	2	0	2	2	4
2538.9877	2538.9872	0.0005	2	2	1	2	3	2	0	2	1	3
2539.3681	2539.3671	0.001	2	2	1	1	1	2	0	2	1	1
2539.4383	2539.4365	0.0018	2	2	1	2	3	2	0	2	2	3
2539.5066	2539.5067	-0.0001	2	2	1	0	2	2	0	2	2	3
2539.6441	2539.6411	0.003	2	2	1	0	2	2	0	2	0	2
2903.8453	2903.851	-0.0057	3	3	1	2	1	3	2	2	2	1
2904.1209	2904.1261	-0.0052	3	3	1	2	2	3	2	2	2	2
2904.2879	2904.2953	-0.0074	3	3	1	1	4	3	2	2	1	4
2904.6467	2904.6521	-0.0054	3	3	1	0	3	3	2	2	2	3
3141.2877	3141.2928	-0.0051	3	1	2	0	3	3	1	3	1	3
3141.3426	3141.3459	-0.0033	3	1	2	2	5	3	1	3	2	5
3141.4949	3141.5003	-0.0054	3	1	2	1	4	3	1	3	1	4
3140.866	3140.8679	-0.0019	3	1	2	2	1	3	1	3	2	1
3140.9358	3140.9334	0.0024	3	1	2	1	3	3	3	1	2	3
3141.0556	3141.0582	-0.0026	3	1	2	2	2	3	1	3	2	2
3142.6952	3142.6994	-0.0042	3	1	2	2	3	3	1	3	2	3
3154.714	3154.7162	-0.0022	3	1	2	2	1	3	0	3	2	1
3154.7861	3154.7839	0.0022	3	1	2	1	3	3	0	3	2	3
3154.9129	3154.9125	0.0004	3	1	2	2	2	3	0	3	2	2

3155.1304	3155.1342	-0.0038	3	1	2	0	3	3	0	3	1	3
3155.1931	3155.1891	0.004	3	1	2	2	5	3	0	3	2	5
3155.348	3155.3485	-0.0005	3	1	2	1	4	3	0	3	1	4
3156.3748	3156.3808	-0.006	3	1	2	2	4	3	0	3	2	4
3156.532	3156.5275	0.0045	3	1	2	2	3	3	0	3	0	3
3220.9408	3220.9453	-0.0045	2	0	2	0	2	1	1	1	1	2
3221.1107	3221.1151	-0.0044	2	0	2	2	3	1	1	1	2	3
3221.3781	3221.3823	-0.0042	2	0	2	2	0	1	1	1	1	1
3221.5312	3221.5289	0.0023	2	0	2	1	3	1	1	1	1	2
3221.767	3221.7688	-0.0018	2	0	2	2	4	1	1	1	2	3
3221.8721	3221.875	-0.0029	2	0	2	1	2	1	1	1	0	1
3295.7731	3295.7723	0.0008	2	1	2	0	2	1	1	1	1	2
3295.9148	3295.9167	-0.0019	2	1	2	2	3	1	1	1	2	3
3296.125	3296.1275	-0.0025	2	1	2	2	1	1	1	1	1	1
3296.2065	3296.2101	-0.0036	2	1	2	2	2	1	1	1	1	1
3296.3887	3296.3924	-0.0037	2	1	2	0	2	1	1	1	2	1
3296.475	3296.4776	-0.0026	2	1	2	1	3	1	1	1	1	2
3296.6859	3296.6847	0.0012	2	1	2	2	4	1	1	1	2	3
3296.7724	3296.7726	-0.0002	2	1	2	1	2	1	1	1	0	1
3297.6252	3297.6318	-0.0066	2	1	2	2	2	1	1	1	2	2
3297.787	3297.7916	-0.0046	2	1	2	2	0	1	1	1	2	1
3483.2447	3483.2415	0.0032	3	2	2	1	3	3	3	1	2	3
3483.1392	3483.1299	0.0093	3	2	2	2	1	3	1	3	2	1
3483.5495	3483.5485	0.001	3	2	2	2	5	3	1	3	2	5
3483.8051	3483.7978	0.0073	3	2	2	1	4	3	1	3	1	4
3484.433	3484.4313	0.0017	3	2	2	1	2	3	1	3	1	2
3484.504	3484.4955	0.0085	3	2	2	2	4	3	1	3	2	4
3484.7095	3484.7048	0.0047	3	2	2	2	3	3	1	3	2	3
3487.1646	3487.1628	0.0018	2	0	2	2	3	1	0	1	2	2
3487.4126	3487.4097	0.0029	2	0	2	1	3	1	0	1	1	2
3487.5345	3487.5383	-0.0038	2	0	2	2	4	1	0	1	2	3
3487.7924	3487.7867	0.0057	2	0	2	2	2	1	0	1	1	1
3496.9809	3496.9781	0.0028	3	2	2	2	1	3	0	3	2	1
3497.0952	3497.092	0.0032	3	2	2	1	3	3	0	3	2	3
3497.3964	3497.3917	0.0047	3	2	2	2	5	3	0	3	2	5
3497.6502	3497.646	0.0042	3	2	2	1	4	3	0	3	1	4
3498.2557	3498.2538	0.0019	3	2	2	1	2	3	0	3	1	2
3498.3285	3498.3189	0.0096	3	2	2	2	4	3	0	3	2	4
3498.5387	3498.5328	0.0059	3	2	2	2	3	3	0	3	0	3
3561.7622	3561.762	0.0002	2	1	2	2	3	1	0	1	1	2
3561.8301	3561.8282	0.0019	2	1	2	0	2	1	0	1	0	1
3561.966	3561.9644	0.0016	2	1	2	2	3	1	0	1	2	2

3562.0922	3562.0847	0.0075	2	1	2	1	1	1	0	1	1	0
3562.1663	3562.1662	0.0001	2	1	2	1	2	1	0	1	2	1
3562.3637	3562.3584	0.0053	2	1	2	1	3	1	0	1	1	2
3562.4539	3562.4542	-0.0003	2	1	2	2	4	1	0	1	2	3
3562.566	3562.5608	0.0052	2	1	2	1	3	1	0	1	2	2
3562.7756	3562.7737	0.0019	2	1	2	2	2	1	0	1	1	1
3562.9226	3562.9186	0.004	2	1	2	2	2	1	0	1	1	2
3660.2284	3660.2251	0.0033	4	3	2	2	4	4	2	3	0	4
3660.3336	3660.3422	-0.0086	4	3	2	2	6	4	2	3	2	6
3660.5262	3660.5278	-0.0016	4	3	2	1	5	4	2	3	1	5
3660.8293	3660.836	-0.0067	4	3	2	2	5	4	2	3	2	5
3661.0097	3661.006	0.0037	4	3	2	0	4	4	2	3	2	4
3990.2202	3990.2242	-0.004	6	3	3	2	8	6	3	4	2	8
3990.8592	3990.8617	-0.0025	6	3	3	2	7	6	3	4	1	7
4199.6128	4199.6045	0.0083	4	1	3	2	4	3	3	0	2	3
4200.2567	4200.2474	0.0093	4	1	3	1	5	3	3	0	1	4
4244.217	4244.2097	0.0073	5	1	4	2	6	4	3	1	2	5
4245.1377	4245.1415	-0.0038	5	1	4	1	6	4	3	1	1	5
4245.3629	4245.3669	-0.004	5	1	4	2	7	4	3	1	2	6
4245.622	4245.6345	-0.0125	5	1	4	0	5	4	3	1	1	4
4245.6904	4245.6934	-0.003	5	1	4	2	3	4	3	1	2	2
4407.5156	4407.5174	-0.0018	2	1	1	1	3	1	1	0	1	2
4407.4303	4407.4341	-0.0038	2	1	1	1	1	1	1	0	1	0
4407.6907	4407.6916	-0.0009	2	1	1	2	4	1	1	0	2	3
4407.8076	4407.8069	0.0007	2	1	1	0	2	1	1	0	1	1
4406.6043	4406.5977	0.0066	2	1	1	1	2	1	1	0	2	2
4626.9832	4626.9908	-0.0076	4	1	3	2	6	4	1	4	2	6
4627.1789	4627.1854	-0.0065	4	1	3	1	5	4	1	4	1	5
4626.755	4626.7529	0.0021	4	1	3	1	4	4	1	4	2	4
4626.7011	4626.7006	0.0005	4	1	3	2	2	4	1	4	2	2
4628.0998	4628.0999	-0.0001	4	1	3	2	4	4	1	4	0	4
4629.0844	4629.097	-0.0126	4	1	3	2	6	4	0	4	2	6
4718.8098	4718.8114	-0.0016	4	2	3	2	2	4	1	4	2	2
4718.875	4718.873	0.002	4	2	3	0	4	4	1	4	2	4
4719.0783	4719.0871	-0.0088	4	2	3	2	6	4	1	4	2	6
4719.2867	4719.2847	0.002	4	2	3	1	5	4	1	4	1	5
4720.1412	4720.1402	0.001	4	2	3	2	4	4	1	4	0	4
4719.9558	4719.9616	-0.0058	4	2	3	2	5	4	1	4	2	5
4720.9158	4720.9181	-0.0023	4	2	3	2	2	4	0	4	2	2
4720.9835	4720.9799	0.0036	4	2	3	0	4	4	2	2	2	4
4721.182	4721.1932	-0.0112	4	2	3	2	6	4	0	4	2	6
4721.3934	4721.3916	0.0018	4	2	3	1	5	4	0	4	1	5

4722.0595	4722.0651	-0.0056	4	2	3	2	5	4	0	4	2	5
4722.2471	4722.2443	0.0028	4	2	3	2	4	4	0	4	2	4
4744.3713	4744.372	-0.0007	3	0	3	1	4	2	1	2	1	3
4744.4545	4744.4547	-0.0002	3	0	3	2	5	2	1	2	2	4
4757.346	4757.351	-0.005	3	1	3	2	4	2	1	2	2	4
4758.0196	4758.0186	0.001	3	1	3	2	3	2	1	2	0	2
4758.119	4758.119	0	3	1	3	2	4	2	1	2	2	3
4758.2242	4758.2203	0.0039	3	1	3	1	4	2	1	2	1	3
4758.3015	4758.2979	0.0036	3	1	3	2	5	2	1	2	2	4
4758.4127	4758.4107	0.002	3	1	3	2	1	2	1	2	2	1
4759.2854	4759.2801	0.0053	3	1	3	2	2	2	1	2	0	2
4759.3757	4759.3731	0.0026	3	3	1	2	3	2	1	2	2	3
4818.4503	4818.4434	0.0069	3	0	3	2	4	2	0	2	2	4
4818.8835	4818.8832	0.0003	3	0	3	0	3	2	0	2	2	3
4819.0183	4819.0175	0.0008	3	0	3	0	3	2	0	2	0	2
4819.0884	4819.0971	-0.0087	3	0	3	2	4	2	0	2	2	3
4819.2385	4819.2399	-0.0014	3	0	3	2	2	2	0	2	2	1
4819.5557	4819.5595	-0.0038	3	0	3	2	1	2	0	2	2	1
4819.6444	4819.6484	-0.004	3	0	3	1	3	2	0	2	1	3
4820.2518	4820.2528	-0.001	3	0	3	2	2	2	0	2	0	2
4820.323	4820.3242	-0.0012	3	0	3	2	3	2	0	2	2	3
4832.7142	4832.7113	0.0029	3	1	3	2	3	2	0	2	2	3
4832.851	4832.8456	0.0054	3	1	3	2	3	2	0	2	0	2
4832.9236	4832.9206	0.003	3	1	3	2	4	2	0	2	2	3
4833.0937	4833.0943	-0.0006	3	1	3	2	2	2	0	2	2	1
4833.2034	4833.2138	-0.0104	3	1	3	2	5	2	0	2	2	4
4833.4112	4833.4078	0.0034	3	1	3	2	1	2	0	2	2	1
4833.4895	4833.4898	-0.0003	3	1	3	1	3	2	0	2	1	3
4834.1104	4834.1072	0.0032	3	1	3	2	2	2	0	2	0	2
4834.1809	4834.1747	0.0062	3	3	1	2	3	2	0	2	2	3
5204.3092	5204.3128	-0.0036	2	2	1	1	3	1	1	0	2	2
5204.4811	5204.4834	-0.0023	2	2	1	2	3	1	1	0	2	2
5204.5542	5204.5536	0.0006	2	2	1	0	2	1	1	0	2	2
5204.6155	5204.6144	0.0011	2	2	1	0	2	1	1	0	0	1
5204.6978	5204.6971	0.0007	2	2	1	2	2	1	1	0	1	2
5204.7777	5204.7789	-0.0012	2	2	1	1	2	1	1	0	1	2
5204.9627	5204.9558	0.0069	2	2	1	2	4	1	1	0	2	3
5205.0986	5205.1011	-0.0025	2	2	1	2	3	1	1	0	1	2
5205.23	5205.2307	-0.0007	2	2	1	2	3	1	1	0	2	3
5205.3087	5205.3096	-0.0009	2	2	1	1	1	1	1	0	1	1
5205.4018	5205.4017	0.0001	2	2	1	0	2	1	1	0	1	1
5205.7657	5205.7696	-0.0039	2	2	1	2	0	1	1	0	2	1

5205.9234	5205.9328	-0.0094	2	2	1	1	2	1	1	0	2	1
5206.2332	5206.2332	0	2	2	1	1	1	1	1	0	2	1
5274.0009	5274.0017	-0.0008	6	5	2	2	7	6	3	3	2	7
5777.9064	5777.9093	-0.0029	3	2	2	2	3	2	2	1	0	2
5777.9768	5777.9795	-0.0027	3	2	2	1	4	2	2	1	2	3
5778.1503	5778.1501	0.0002	3	2	2	2	4	2	2	1	1	3
5778.2672	5778.2545	0.0127	3	2	2	2	5	2	2	1	2	4
5778.3751	5778.3836	-0.0085	3	2	2	0	3	2	2	1	2	2
5916.1043	5916.1117	-0.0074	6	2	4	2	7	6	2	5	1	7
5915.9958	5916.0065	-0.0107	6	2	4	2	8	6	2	5	2	8
5915.9958	5916.0056	-0.0098	6	2	4	1	5	6	2	5	2	5
5915.9125	5915.9101	0.0024	6	0	6	0	6	6	4	3	2	6
5916.613	5916.622	-0.009	6	2	4	1	7	6	2	5	2	7
5916.7048	5916.7141	-0.0093	6	4	2	2	6	6	2	5	2	6
6006.1625	6006.1516	0.0109	6	5	2	2	6	6	1	5	0	6
6006.0538	6006.0401	0.0137	6	3	4	1	7	6	1	5	2	7
6005.6092	6005.5964	0.0128	6	3	4	2	7	6	1	5	1	7
6025.2114	6025.2107	0.0007	5	1	4	2	7	5	1	5	2	7
6025.2114	6025.2128	-0.0014	5	1	4	2	4	5	1	5	2	4
6025.3751	6025.3767	-0.0016	5	1	4	1	6	5	1	5	1	6
6026.1536	6026.1572	-0.0036	5	1	4	2	5	5	1	5	2	5
6026.0037	6026.0018	0.0019	5	1	4	2	6	5	1	5	2	6
6043.686	6043.6897	-0.0037	5	2	4	0	5	5	0	5	2	5
6043.8474	6043.8417	0.0057	5	2	4	2	7	5	0	5	2	7
6044.0155	6044.0114	0.0041	5	2	4	1	6	5	0	5	1	6
6044.6193	6044.6172	0.0021	5	2	4	2	6	5	0	5	2	6
6044.7791	6044.7763	0.0028	5	2	4	2	5	5	0	5	0	5
6151.7333	6151.7369	-0.0036	4	1	4	2	5	3	1	3	2	5
6150.7038	6150.7124	-0.0086	4	0	4	2	6	3	1	3	2	5
6152.6807	6152.6838	-0.0031	4	1	4	2	5	3	1	3	2	4
6152.8074	6152.8185	-0.0111	4	1	4	2	6	3	1	3	2	5
6152.9577	6152.9567	0.001	4	1	4	1	3	3	1	3	2	3
6153.064	6153.0666	-0.0026	4	1	4	2	2	3	1	3	2	2
6153.1351	6153.1322	0.0029	4	1	4	1	4	3	1	3	1	4
6164.1408	6164.1374	0.0034	4	0	4	2	4	3	0	3	2	4
6163.4723	6163.4765	-0.0042	4	0	4	2	5	3	0	3	2	5
6164.4088	6164.4038	0.005	4	0	4	2	5	3	0	3	2	4
6164.5548	6164.5555	-0.0007	4	0	4	2	6	3	0	3	2	5
6164.8713	6164.8745	-0.0032	4	0	4	1	4	3	0	3	1	4
6166.504	6166.5073	-0.0033	4	1	4	2	5	3	0	3	2	4
6232.9651	6232.9757	-0.0106	3	1	2	2	4	2	1	1	2	3
6233.3089	6233.3161	-0.0072	3	1	2	2	5	2	1	1	2	4

6233.5496	6233.5573	-0.0077	3	1	2	1	3	2	1	1	1	2
6389.8124	6389.814	-0.0016	2	2	0	2	0	1	0	1	2	1
6389.9728	6389.9731	-0.0003	2	2	0	2	2	1	0	1	2	1
6390.0639	6390.0658	-0.0019	2	2	0	2	1	1	0	1	2	1
6390.2	6390.2014	-0.0014	2	2	0	1	2	1	0	1	2	1
6390.2673	6390.2628	0.0045	2	2	0	2	2	1	0	1	1	1
6390.4946	6390.491	0.0036	2	2	0	1	2	1	0	1	1	1
6390.6464	6390.6492	-0.0028	2	2	0	2	4	1	0	1	2	3
6390.9335	6390.9295	0.004	2	2	0	1	3	1	0	1	1	2
6391.1343	6391.1319	0.0024	2	2	0	1	3	1	0	1	2	2
6391.3022	6391.303	-0.0008	2	2	0	2	3	1	0	1	2	3
6391.3822	6391.3788	0.0034	2	2	0	2	3	1	0	1	1	2
6391.581	6391.5812	-0.0002	2	2	0	2	3	1	0	1	2	2
6391.6838	6391.6883	-0.0045	2	2	0	0	2	1	0	1	0	1
6574.9144	6574.9138	0.0006	3	2	2	2	4	2	1	1	2	3
6575.8602	6575.8653	-0.0051	3	2	2	1	3	2	1	1	1	2
6736.8923	6736.8793	0.013	3	2	1	1	4	2	2	0	1	3
6737.0843	6737.0659	0.0184	3	2	1	2	5	2	2	0	2	4
7388.0629	7388.0627	0.0002	4	2	3	2	4	3	2	2	2	3
7388.1483	7388.1499	-0.0016	4	2	3	2	5	3	2	2	2	4
7388.2687	7388.2624	0.0063	4	2	3	1	5	3	2	2	1	4
7389.0185	7389.0183	0.0002	6	1	5	1	7	6	1	6	1	7
7389.6977	7389.6991	-0.0014	6	1	5	0	6	6	1	6	2	6
7392.1508	7392.1555	-0.0047	6	2	5	1	7	6	0	6	1	7
7392.0177	7392.0046	0.0131	6	2	5	2	8	6	0	6	2	8
7391.8988	7391.8927	0.0061	6	4	3	2	6	6	2	4	2	6
7392.8312	7392.8339	-0.0027	6	2	5	2	6	6	0	6	2	6
7527.6898	7527.6907	-0.0009	5	1	5	2	7	4	1	4	2	6
7638.5945	7638.5933	0.0012	4	1	3	1	4	3	1	2	1	3
7730.0947	7730.088	0.0067	4	2	3	2	5	3	1	2	2	4
7730.568	7730.5597	0.0083	4	2	3	2	6	3	1	2	2	5
7730.7167	7730.7134	0.0033	4	2	3	0	4	3	1	2	1	3
6164.8172	6164.8143	0.0029	4	0	4	2	2	3	0	3	2	2
6164.6857	6164.6813	0.0044	4	0	4	1	3	3	0	3	0	3
7388.3545	7388.3571	-0.0026	4	2	3	2	6	3	2	2	2	5
6025.0547	6025.0555	-0.0008	5	1	4	0	5	5	3	3	2	5
3222.825	3222.8302	-0.0052	2	0	2	2	0	1	1	1	2	1
3222.6405	3222.6449	-0.0044	2	0	2	2	2	1	1	1	2	2
3222.4397	3222.4425	-0.0028	2	0	2	1	2	1	1	1	2	1
3221.2178	3221.2231	-0.0053	2	0	2	2	2	1	1	1	1	1
2904.4518	2904.4524	-0.0006	3	3	1	2	4	3	2	2	2	4
2903.9641	2903.9563	0.0078	3	1	3	0	3	3	2	2	0	3

3221.675	3221.6736	0.0014	2	0	2	2	3	1	1	1	2	2
4304.7612	4304.7542	0.007	5	4	2	2	5	5	2	3	2	5
4304.5625	4304.552	0.0105	5	4	2	2	6	5	2	3	2	6
4304.4875	4304.4902	-0.0027	5	4	2	2	7	5	2	3	2	7
2606.4375	2606.4358	0.0017	5	3	2	2	7	5	2	3	2	7
2606.4875	2606.4842	0.0033	5	3	2	1	6	5	2	3	1	6
2539.575	2539.5708	0.0042	2	2	1	2	3	2	0	2	0	2
2539.2625	2539.2659	-0.0034	2	2	1	1	3	2	0	2	2	3
2649.2281	2649.2238	0.0043	8	5	3	2	10	8	5	4	2	10
2649.6873	2649.6933	-0.006	8	5	3	2	9	8	5	4	2	9
2779.4923	2779.4994	-0.0071	4	2	2	2	5	4	2	3	2	5
2778.6524	2778.6465	0.0059	4	2	2	2	6	4	2	3	2	6
3246.2651	3246.2689	-0.0038	3	3	1	2	5	3	1	2	2	5
3246.1402	3246.1404	-0.0002	3	1	3	0	3	3	1	2	0	3
3246.5869	3246.5928	-0.0059	3	3	1	1	4	3	1	2	1	4
3246.6569	3246.6575	-0.0006	3	3	1	0	3	3	1	2	2	3
3246.39	3246.3905	-0.0005	3	3	1	2	4	3	1	2	2	4
3382.9868	3382.9844	0.0024	7	4	3	1	7	7	4	4	1	7
3383.0691	3383.0651	0.004	7	4	3	2	9	7	4	4	2	9
3383.6243	3383.6227	0.0016	7	4	3	2	8	7	4	4	2	8
3753.0514	3753.0463	0.0051	4	3	2	0	4	4	1	3	2	4
3972.8403	3972.8381	0.0022	5	4	2	2	5	5	5	1	2	5
3972.6811	3972.684	-0.0029	5	4	2	2	6	5	3	3	2	6
3990.1148	3990.1154	-0.0006	6	3	3	1	6	6	1	6	0	6
4405.7212	4405.7191	0.0021	5	2	3	1	6	5	2	4	1	6
4406.3738	4406.3771	-0.0033	5	2	3	2	6	5	2	4	2	6
4406.4548	4406.4612	-0.0064	5	2	3	2	5	5	2	4	2	5
4424.7901	4424.7916	-0.0015	5	2	3	2	5	5	1	4	2	5
4424.7014	4424.7039	-0.0025	5	2	3	2	6	5	1	4	2	6
4424.0618	4424.0647	-0.0029	5	2	3	1	6	5	1	4	1	6
7321.2878	7321.2801	0.0077	7	2	5	1	8	7	2	6	1	8
7321.1689	7321.1683	0.0006	7	2	5	2	9	7	2	6	2	9
7321.0927	7321.0932	-0.0005	7	2	5	0	7	7	4	4	2	7
7321.806	7321.8099	-0.0039	7	0	7	0	7	7	2	6	2	7
7321.7068	7321.7021	0.0047	7	2	5	2	8	7	2	6	2	8
7339.5944	7339.5949	-0.0005	7	3	5	1	8	7	1	6	1	8
7339.9996	7340.0053	-0.0057	7	3	5	2	8	7	1	6	2	8
7340.1151	7340.1149	0.0002	7	5	3	2	7	7	1	6	2	7
7339.475	7339.4814	-0.0064	7	3	5	2	9	7	1	6	2	9
7529.5141	7529.5078	0.0063	5	0	5	2	7	4	0	4	2	6
7638.4638	7638.4634	0.0004	4	1	3	2	6	3	1	2	2	5

Table S12: List of lines assigned for the C1 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2535.1429	2535.1502	-0.0073	2	2	1	3	4	2	0	2	3	4
2534.9227	2534.9296	-0.0069	2	2	1	1	2	2	0	2	1	2
2535.45	2535.4578	-0.0078	2	2	1	3	3	2	0	2	2	3
2535.6298	2535.6335	-0.0037	2	2	1	2	3	2	0	2	2	3
3486.4084	3486.4051	0.0033	2	0	2	3	4	1	0	1	2	3
3486.2798	3486.2764	0.0034	2	0	2	2	3	1	0	1	2	2
3486.0342	3486.0321	0.0021	2	0	2	3	3	1	0	1	1	2
3495.3566	3495.358	-0.0014	3	2	2	3	4	3	0	3	3	4
3495.1019	3495.1059	-0.004	3	2	2	4	5	3	0	3	4	5
3496.0406	3496.035	0.0056	3	2	2	4	4	3	0	3	4	4
3496.2433	3496.2468	-0.0035	3	2	2	3	3	3	0	3	3	3
3495.9732	3495.9703	0.0029	3	2	2	2	2	3	0	3	2	2
3560.7495	3560.7412	0.0083	2	1	2	3	4	1	0	1	2	3
3560.6404	3560.6472	-0.0068	2	1	2	2	3	1	0	1	2	2
3748.6118	3748.6105	0.0013	4	3	2	4	4	4	1	3	4	4
4295.5087	4295.5184	-0.0097	5	4	2	6	5	5	2	3	6	5
4295.5871	4295.5845	0.0026	5	4	2	6	6	5	2	3	6	6
4295.8031	4295.7909	0.0122	5	4	2	5	5	5	2	3	5	5
4295.7597	4295.7439	0.0158	5	4	2	5	6	5	2	3	5	6
4743.3804	4743.3843	-0.0039	3	0	3	2	3	2	1	2	1	2
4743.3018	4743.2986	0.0032	3	0	3	3	4	2	1	2	2	3
4743.125	4743.1169	0.0081	3	0	3	3	3	2	1	2	2	2
4757.0716	4757.0656	0.006	3	1	3	2	3	2	1	2	1	2
4756.9939	4756.9872	0.0067	3	1	3	3	4	2	1	2	2	3
4817.4413	4817.4432	-0.0019	3	0	3	4	4	2	0	2	3	3
4817.3689	4817.3655	0.0034	3	0	3	3	3	2	0	2	2	2
4817.2328	4817.2314	0.0014	3	0	3	3	3	2	0	2	3	3
4817.5882	4817.5886	-0.0004	3	0	3	3	2	2	0	2	2	1
4817.9075	4817.9053	0.0022	3	0	3	2	1	2	0	2	2	1
4817.6918	4817.7011	-0.0093	3	0	3	2	3	2	0	2	1	2
5201.3993	5201.3911	0.0082	2	2	1	3	4	1	1	0	2	3
5777.6893	5777.6731	0.0162	3	2	2	4	5	2	2	1	3	4
5777.5728	5777.5696	0.0032	3	2	2	4	4	2	2	1	3	3
5777.5728	5777.5696	0.0032	3	2	2	3	4	2	2	1	3	3
5777.3977	5777.3939	0.0038	3	2	2	3	4	2	2	1	2	3

5777.3977	5777.3939	0.0038	3	2	2	4	4	2	2	1	2	3
5777.3977	5777.3939	0.0038	3	2	2	3	3	2	2	1	2	3
5777.3285	5777.3244	0.0041	3	2	2	3	3	2	2	1	2	2
5777.793	5777.8048	-0.0118	3	2	2	2	3	2	2	1	1	2
6041.7257	6041.7254	0.0003	5	2	4	6	7	5	0	5	6	7
6041.8912	6041.8915	-0.0003	5	2	4	5	6	5	0	5	5	6
6041.5725	6041.5729	-0.0004	5	2	4	6	5	5	0	5	6	5
6042.6575	6042.6582	-0.0007	5	2	4	5	5	5	0	5	5	5
6042.4942	6042.5026	-0.0084	5	2	4	6	6	5	0	5	6	6
6151.0293	6151.0404	-0.0111	4	1	4	5	6	3	1	3	4	5
6150.9051	6150.9053	-0.0002	4	1	4	5	5	3	1	3	4	4
6150.8483	6150.8496	-0.0013	4	1	4	4	4	3	1	3	3	3
6162.5011	6162.4975	0.0036	4	0	4	5	5	3	0	3	4	4
6231.4686	6231.4785	-0.0099	3	1	2	4	4	2	1	1	3	3
6231.8196	6231.8204	-0.0008	3	1	2	4	5	2	1	1	3	4
6231.7674	6231.772	-0.0046	3	1	2	3	4	2	1	1	2	3
6232.0549	6232.0634	-0.0085	3	1	2	4	3	2	1	1	3	2
6386.901	6386.9038	-0.0028	2	2	0	3	4	1	0	1	2	3
6387.1846	6387.1833	0.0013	2	2	0	2	3	1	0	1	2	2
6387.6355	6387.634	0.0015	2	2	0	3	3	1	0	1	2	2
6387.3962	6387.3898	0.0064	2	2	0	2	3	1	0	1	1	2
7386.5299	7386.5249	0.005	4	2	3	4	4	3	2	2	3	3
7386.6139	7386.6124	0.0015	4	2	3	5	5	3	2	2	4	4
7386.7409	7386.7248	0.0161	4	2	3	4	5	3	2	2	3	4
7386.8089	7386.8199	-0.011	4	2	3	5	6	3	2	2	4	5
7525.4758	7525.4733	0.0025	5	1	5	6	7	4	1	4	5	6
7525.3686	7525.371	-0.0024	5	1	5	4	4	4	1	4	3	3
7525.4391	7525.4452	-0.0061	5	1	5	5	6	4	1	4	4	5
7635.6205	7635.6233	-0.0028	4	1	3	5	4	3	1	2	4	3
7635.6205	7635.6273	-0.0068	4	1	3	3	3	3	1	2	3	2
7635.4902	7635.492	-0.0018	4	1	3	5	6	3	1	2	4	5
7635.1161	7635.1279	-0.0118	4	1	3	5	5	3	1	2	4	4
7635.0561	7635.0563	-0.0002	4	1	3	4	4	3	1	2	3	3
2781.03	2781.023	0.007	4	2	2	4	5	4	2	3	4	5
6162.6425	6162.6497	-0.0072	4	0	4	5	6	3	0	3	4	5
2278.7474	2278.7407	0.0067	5	3	2	5	4	5	3	3	5	4
2279.5183	2279.5153	0.003	5	3	2	5	5	5	3	3	5	5
2781.8441	2781.8387	0.0054	4	2	2	5	5	4	2	3	5	5
2536.2867	2536.2878	-0.0011	2	2	1	2	2	2	0	2	2	2
2536.0787	2536.0843	-0.0056	2	2	1	2	3	2	0	2	3	3
2536.1526	2536.1537	-0.0011	2	2	1	2	2	2	0	2	3	3
2780.7893	2780.7993	-0.01	4	2	2	4	3	4	2	3	4	3

3494.8056	3494.8054	0.0002	3	2	2	4	3	3	0	3	4	3
4831.1139	4831.1068	0.0071	3	1	3	4	4	2	0	2	3	3
4831.0399	4831.0339	0.006	3	1	3	3	3	2	0	2	2	2
4831.2822	4831.2832	-0.001	3	1	3	3	2	2	0	2	2	1
4831.3829	4831.3824	0.0005	3	1	3	2	3	2	0	2	1	2

Table S13: List of lines assigned for the C2 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2516.1358	2516.1395	-0.0037	2	2	1	3	4	2	0	2	3	4
2783.046	2783.0471	-0.0011	4	2	2	4	5	4	2	3	4	5
2782.99	2782.9974	-0.0074	4	2	2	5	6	4	2	3	5	6
2783.8043	2783.8074	-0.0031	4	2	2	5	5	4	2	3	5	5
3284.2403	3284.235	0.0053	2	1	2	3	4	1	1	1	2	3
3284.3199	3284.3217	-0.0018	2	1	2	1	2	1	1	1	0	1
3471.9709	3471.9717	-0.0008	2	0	2	3	4	1	0	1	2	3
3471.8651	3471.8629	0.0022	2	0	2	2	3	1	0	1	2	2
3471.6011	3471.6018	-0.0007	2	0	2	3	3	1	0	1	1	2
3477.5129	3477.5195	-0.0066	3	2	2	4	3	3	0	3	4	3
3477.8165	3477.821	-0.0045	3	2	2	4	5	3	0	3	4	5
3477.7478	3477.7482	-0.0004	3	2	2	2	3	3	0	3	2	3
3478.0718	3478.0738	-0.002	3	2	2	3	4	3	0	3	3	4
3478.9669	3478.9657	0.0012	3	2	2	3	3	3	0	3	3	3
3478.7581	3478.7532	0.0049	3	2	2	4	4	3	0	3	4	4
3478.6884	3478.6884	0	3	2	2	2	2	3	0	3	2	2
3722.1712	3722.1682	0.003	4	3	2	4	5	4	1	3	5	5
3722.4246	3722.4248	-0.0002	4	3	2	5	5	4	1	3	4	5
4394.4254	4394.4248	0.0006	2	1	1	3	4	1	1	0	2	3
4394.54	4394.5389	0.0011	2	1	1	1	2	1	1	0	0	1
4394.2428	4394.2531	-0.0103	2	1	1	2	3	1	1	0	1	2
4395.1367	4395.1261	0.0106	2	1	1	3	2	1	1	0	2	1
4738.3753	4738.374	0.0013	3	1	3	4	5	2	1	2	3	4
4738.2943	4738.2969	-0.0026	3	1	3	3	4	2	1	2	2	3
4738.1884	4738.1905	-0.0021	3	1	3	4	4	2	1	2	3	3
4738.0931	4738.0908	0.0023	3	1	3	3	3	2	1	2	2	2
4797.2981	4797.2845	0.0136	3	0	3	4	5	2	0	2	3	4
4797.2373	4797.2348	0.0025	3	0	3	3	4	2	0	2	2	3
4797.1491	4797.1476	0.0015	3	0	3	3	2	2	0	2	2	1
4797.0169	4797.0221	-0.0052	3	0	3	4	4	2	0	2	3	3
4796.9403	4796.9426	-0.0023	3	0	3	3	3	2	0	2	2	2

4796.8097	4796.8096	0.0001	3	0	3	3	3	2	0	2	3	3
4797.4628	4797.4653	-0.0025	3	0	3	2	1	2	0	2	2	1
4797.5653	4797.5604	0.0049	3	0	3	2	3	2	0	2	2	3
4798.179	4798.1844	-0.0054	3	0	3	3	2	2	0	2	2	2
4798.2496	4798.2559	-0.0063	3	0	3	4	3	2	0	2	3	3
5758.8389	5758.8332	0.0057	3	2	2	4	4	2	2	1	3	3
5758.8389	5758.8332	0.0057	3	2	2	3	4	2	2	1	3	3
5758.9691	5758.966	0.0031	3	2	2	4	5	2	2	1	3	4
5758.6726	5758.6767	-0.0041	3	2	2	3	4	2	2	1	2	3
5758.6726	5758.6768	-0.0042	3	2	2	4	4	2	2	1	2	3
5758.6726	5758.6768	-0.0042	3	2	2	3	3	2	2	1	2	3
5758.5923	5758.5851	0.0072	3	2	2	3	3	2	2	1	2	2
6126.0838	6126.0887	-0.0049	4	1	4	5	6	3	1	3	4	5
6125.9501	6125.9546	-0.0045	4	1	4	5	5	3	1	3	4	4
6137.1742	6137.1899	-0.0157	4	0	4	5	6	3	0	3	4	5
6137.0412	6137.0417	-0.0005	4	0	4	5	5	3	0	3	4	4
6720.3894	6720.3806	0.0088	3	2	1	3	4	2	2	0	2	3
6720.5667	6720.5647	0.002	3	2	1	4	5	2	2	0	3	4
7359.442	7359.4259	0.0161	4	2	3	4	4	3	2	2	3	3
7359.5139	7359.5124	0.0015	4	2	3	5	5	3	2	2	4	4
7359.6406	7359.6358	0.0048	4	2	3	4	5	3	2	2	3	4
7359.7131	7359.7298	-0.0167	4	2	3	5	6	3	2	2	4	5
7359.7807	7359.7808	-0.0001	4	2	3	5	4	3	2	2	4	3
7494.722	7494.7131	0.0089	5	1	5	6	7	4	1	4	5	6
7494.6093	7494.6169	-0.0076	5	1	5	6	6	4	1	4	5	5
7494.675	7494.6846	-0.0096	5	1	5	5	6	4	1	4	4	5
7496.4112	7496.3996	0.0116	5	0	5	6	7	4	0	4	5	6
7496.2987	7496.3015	-0.0028	5	0	5	6	6	4	0	4	5	5
7496.3625	7496.352	0.0105	5	0	5	4	3	4	0	4	3	2
7602.3099	7602.3181	-0.0082	4	1	3	5	6	3	1	2	4	5
7602.4316	7602.4352	-0.0036	4	1	3	5	4	3	1	2	4	3
7601.9366	7601.9339	0.0027	4	1	3	5	5	3	1	2	4	4
3721.871	3721.8679	0.0031	4	3	2	5	4	4	1	3	5	4
3721.8103	3721.8065	0.0038	4	3	2	3	2	4	1	3	3	2
3721.974	3721.9729	0.0011	4	3	2	5	6	4	1	3	5	6
4809.9832	4809.9809	0.0023	3	1	3	3	3	2	0	2	2	2
4810.3122	4810.318	-0.0058	3	1	3	2	3	2	0	2	1	2

Table S14: List of lines assigned for the C3 isotopologue of 2-NBN.

Observed	Calculated	Obs- <i>Calc</i>	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
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[MHz]	[MHz]	[MHz]										
2703.5734	2703.5684	0.005	4	2	2	4	3	4	2	3	4	3
2704.5919	2704.59	0.0019	4	2	2	4	4	4	2	3	4	4
3090.3514	3090.3637	-0.0123	3	1	2	4	5	3	1	3	4	5
3090.508	3090.5058	0.0022	3	1	2	3	4	3	1	3	3	4
3090.0732	3090.0743	-0.0011	3	1	2	3	2	3	1	3	3	2
3260.9335	3260.9297	0.0038	2	1	2	3	4	1	1	1	2	3
3260.1603	3260.1591	0.0012	2	1	2	3	3	1	1	1	2	3
3260.5375	3260.5362	0.0013	2	1	2	3	2	1	1	1	1	1
3456.8004	3456.7984	0.002	2	0	2	3	4	1	0	1	2	3
3456.6943	3456.6939	0.0004	2	0	2	2	3	1	0	1	2	2
3456.2684	3456.2764	-0.008	2	0	2	2	2	1	0	1	1	1
3456.4395	3456.4422	-0.0027	2	0	2	3	3	1	0	1	1	2
3457.0272	3457.0269	0.0003	2	0	2	3	2	1	0	1	2	1
3481.3849	3481.386	-0.0011	3	2	2	4	4	3	0	3	4	4
4324.3194	4324.3274	-0.008	5	2	3	5	5	5	2	4	5	5
4324.251	4324.2518	-0.0008	5	2	3	6	6	5	2	4	6	6
4323.4541	4323.4484	0.0057	5	2	3	5	4	5	2	4	5	4
4323.5331	4323.5228	0.0103	5	2	3	6	7	5	2	4	6	7
4323.5909	4323.5995	-0.0086	5	2	3	5	6	5	2	4	5	6
4323.3716	4323.3758	-0.0042	5	2	3	6	5	5	2	4	6	5
4349.976	4349.9855	-0.0095	2	1	1	3	4	1	1	0	2	3
4350.0887	4350.1006	-0.0119	2	1	1	1	2	1	1	0	0	1
4349.8003	4349.8057	-0.0054	2	1	1	2	3	1	1	0	1	2
4712.4386	4712.4351	0.0035	3	1	3	4	5	2	1	2	3	4
4712.3611	4712.3577	0.0034	3	1	3	3	4	2	1	2	2	3
4712.2433	4712.2507	-0.0074	3	1	3	4	4	2	1	2	3	3
4712.1549	4712.1511	0.0038	3	1	3	3	3	2	1	2	2	2
4712.5501	4712.5458	0.0043	3	1	3	2	1	2	1	2	2	1
4712.6813	4712.6737	0.0076	3	1	3	2	3	2	1	2	2	3
4713.4242	4713.4235	0.0007	3	1	3	3	2	2	1	2	2	2
4713.5176	4713.516	0.0016	3	1	3	4	3	2	1	2	3	3
4711.4803	4711.48	0.0003	3	1	3	4	4	2	1	2	3	4
4778.8619	4778.8495	0.0124	3	0	3	4	5	2	0	2	3	4
4778.815	4778.803	0.012	3	0	3	3	4	2	0	2	2	3
4778.7169	4778.7156	0.0013	3	0	3	3	2	2	0	2	2	1
4778.5811	4778.5844	-0.0033	3	0	3	4	4	2	0	2	3	3
4778.5139	4778.5075	0.0064	3	0	3	3	3	2	0	2	2	2
4778.3784	4778.373	0.0054	3	0	3	3	3	2	0	2	3	3
4779.0341	4779.0318	0.0023	3	0	3	2	1	2	0	2	2	1
4779.1336	4779.127	0.0066	3	0	3	2	3	2	0	2	2	3
5707.7595	5707.7523	0.0072	3	2	2	3	3	2	2	1	2	2

5707.8504	5707.8509	-0.0005	3	2	2	3	4	2	2	1	2	3
5707.8504	5707.8509	-0.0005	3	2	2	4	4	2	2	1	2	3
5707.8504	5707.8509	-0.0005	3	2	2	3	3	2	2	1	2	3
5708.0164	5708.0114	0.005	3	2	2	4	4	2	2	1	3	3
5708.0164	5708.0114	0.005	3	2	2	3	4	2	2	1	3	3
5708.1564	5708.1538	0.0026	3	2	2	4	5	2	2	1	3	4
5708.2892	5708.288	0.0012	3	2	2	2	3	2	2	1	1	2
5964.032	5964.0312	0.0008	5	1	4	6	7	5	1	5	6	7
5964.1932	5964.1905	0.0027	5	1	4	5	6	5	1	5	5	6
5963.8627	5963.8763	-0.0136	5	1	4	6	5	5	1	5	6	5
5986.887	5986.8832	0.0038	5	2	4	6	7	5	0	5	6	7
5987.0589	5987.0472	0.0117	5	2	4	5	6	5	0	5	5	6
5986.7282	5986.7317	-0.0035	5	2	4	6	5	5	0	5	6	5
6096.4302	6096.4491	-0.0189	4	1	4	5	6	3	1	3	4	5
6096.3012	6096.3143	-0.0131	4	1	4	5	5	3	1	3	4	4
6096.3012	6096.3136	-0.0124	4	1	4	3	3	3	1	3	2	2
6109.9666	6109.979	-0.0124	4	0	4	5	6	3	0	3	4	5
6109.8297	6109.828	0.0017	4	0	4	5	5	3	0	3	4	4
6169.0549	6169.0706	-0.0157	3	1	2	4	4	2	1	1	3	3
6169.384	6169.3889	-0.0049	3	1	2	4	5	2	1	1	3	4
6169.6023	6169.6099	-0.0076	3	1	2	4	3	2	1	1	3	2
6637.1845	6637.1797	0.0048	3	2	1	3	4	2	2	0	2	3
6637.3762	6637.3747	0.0015	3	2	1	4	5	2	2	0	3	4
6637.4405	6637.4195	0.021	3	2	1	4	4	2	2	0	3	3
7459.5905	7459.5753	0.0152	5	1	5	6	7	4	1	4	5	6
7459.4765	7459.4781	-0.0016	5	1	5	6	6	4	1	4	5	5
7461.8008	7461.7908	0.01	5	0	5	6	7	4	0	4	5	6
7461.6857	7461.6913	-0.0056	5	0	5	6	6	4	0	4	5	5
7577.6975	7577.7022	-0.0047	4	1	3	5	6	3	1	2	4	5
7577.6975	7577.6996	-0.0021	4	1	3	5	5	3	1	2	3	4
7577.8209	7577.8236	-0.0027	4	1	3	5	4	3	1	2	4	3
2703.7776	2703.7801	-0.0025	4	2	2	4	5	4	2	3	4	5
3091.5144	3091.5146	-0.0002	3	1	2	2	2	3	1	3	2	2
3261.0146	3261.0182	-0.0036	2	1	2	1	2	1	1	1	0	1
3260.6526	3260.6619	-0.0093	2	1	2	3	3	1	1	1	2	2
3260.6526	3260.6636	-0.011	2	1	2	1	1	1	1	1	1	0
3261.8171	3261.8233	-0.0062	2	1	2	3	2	1	1	1	2	2
3456.1255	3456.1272	-0.0017	2	0	2	3	3	1	0	1	2	3
3480.7056	3480.7013	0.0043	3	2	2	3	4	3	0	3	3	4
3480.4529	3480.4497	0.0032	3	2	2	4	5	3	0	3	4	5
3480.3792	3480.3773	0.0019	3	2	2	2	3	3	0	3	2	3
3480.3792	3480.3773	0.0019	3	2	2	3	3	3	0	3	2	3

3480.1442	3480.1466	-0.0024	3	2	2	4	3	3	0	3	4	3
3539.342	3539.3337	0.0083	2	1	2	3	4	1	0	1	2	3
3538.6622	3538.6637	-0.0015	2	1	2	3	3	1	0	1	2	2
3538.7505	3538.7402	0.0103	2	1	2	2	2	1	0	1	1	1
3539.2727	3539.2661	0.0066	2	1	2	2	3	1	0	1	2	2
4696.2323	4696.2309	0.0014	3	0	3	3	4	2	1	2	2	3
4696.2323	4696.2266	0.0057	3	0	3	4	3	2	1	2	3	2
4696.0424	4696.0437	-0.0013	3	0	3	3	3	2	1	2	2	2
4696.3125	4696.3142	-0.0017	3	0	3	4	5	2	1	2	3	4
4779.8201	4779.8239	-0.0038	3	0	3	4	3	2	0	2	3	3
4779.7554	4779.7547	0.0007	3	0	3	3	2	2	0	2	2	2
5987.8061	5987.8091	-0.003	5	2	4	5	5	5	0	5	5	5
5987.6599	5987.6554	0.0045	5	2	4	6	6	5	0	5	6	6
4680.7976	4680.8069	-0.0093	4	2	3	5	6	4	0	4	5	6
4681.0065	4680.9996	0.0069	4	2	3	4	5	4	0	4	4	5
4680.5944	4680.5941	0.0003	4	2	3	5	4	4	0	4	5	4
2551.1458	2551.1454	0.0004	2	2	1	3	4	2	0	2	3	4
3089.9627	3089.9585	0.0042	3	1	2	4	3	3	1	3	4	3

Table S15: List of lines assigned for the C4 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
3074.6562	3074.6502	0.006	3	1	2	4	3	3	1	3	4	3
3075.2263	3075.2287	-0.0024	3	1	2	3	4	3	1	3	3	4
3075.0732	3075.0731	0.0001	3	1	2	4	5	3	1	3	4	5
3075.0269	3075.0203	0.0066	3	1	2	2	3	3	1	3	2	3
3076.3096	3076.3157	-0.0061	3	1	2	4	4	3	1	3	4	4
3255.3494	3255.3471	0.0023	2	1	2	3	4	1	1	1	2	3
3255.4354	3255.4344	0.001	2	1	2	1	2	1	1	1	0	1
3254.84	3254.846	-0.006	2	1	2	3	2	1	1	1	1	1
3254.7577	3254.7629	-0.0052	2	1	2	2	1	1	1	1	1	1
3254.578	3254.5786	-0.0006	2	1	2	3	3	1	1	1	2	3
3256.3097	3256.3134	-0.0037	2	1	2	3	2	1	1	1	2	2
3255.1451	3255.1418	0.0033	2	1	2	2	3	1	1	1	1	2
3255.0696	3255.0701	-0.0005	2	1	2	2	2	1	1	1	2	1
3454.7466	3454.7369	0.0097	2	0	2	3	4	1	0	1	2	3
3454.0966	3454.1022	-0.0056	2	0	2	3	3	1	0	1	2	3
3454.3744	3454.3694	0.005	2	0	2	3	3	1	0	1	1	2
3454.9913	3454.9852	0.0061	2	0	2	3	2	1	0	1	2	1
3542.0711	3542.069	0.0021	2	1	2	3	4	1	0	1	2	3

3541.961	3541.9626	-0.0016	2	1	2	2	3	1	0	1	2	2
4337.6089	4337.6018	0.0071	2	1	1	3	2	1	1	0	2	1
4337.0525	4337.0488	0.0037	2	1	1	1	2	1	1	0	0	1
4336.9335	4336.9338	-0.0003	2	1	1	3	4	1	1	0	2	3
4336.7637	4336.7624	0.0013	2	1	1	2	3	1	1	0	1	2
4336.6881	4336.6933	-0.0052	2	1	1	1	1	1	1	0	1	0
4335.8347	4335.8289	0.0058	2	1	1	3	2	1	1	0	2	2
4560.1102	4560.1111	-0.0009	4	1	3	5	6	4	1	4	5	6
4559.8701	4559.8692	0.0009	4	1	3	5	4	4	1	4	5	4
4561.2498	4561.2438	0.006	4	1	3	4	4	4	1	4	4	4
4678.8222	4678.8259	-0.0037	4	2	3	5	6	4	0	4	5	6
4679.7012	4679.7014	-0.0002	4	2	3	5	5	4	0	4	5	5
4689.7307	4689.7241	0.0066	3	0	3	3	3	2	1	2	2	2
4689.9785	4689.9791	-0.0006	3	0	3	4	5	2	1	2	3	4
4689.891	4689.8953	-0.0043	3	0	3	3	4	2	1	2	2	3
4689.831	4689.8305	0.0005	3	0	3	4	4	2	1	2	3	3
4707.2792	4707.2808	-0.0016	3	1	3	3	3	2	1	2	2	2
4707.3774	4707.3821	-0.0047	3	1	3	4	4	2	1	2	3	3
4707.6664	4707.6682	-0.0018	3	1	3	2	1	2	1	2	2	1
4707.4778	4707.4776	0.0002	3	1	3	3	4	2	1	2	2	3
4707.5565	4707.5559	0.0006	3	1	3	4	5	2	1	2	3	4
4707.1719	4707.1711	0.0008	3	1	3	3	3	2	1	2	3	3
4708.5326	4708.5362	-0.0036	3	1	3	3	2	2	1	2	2	2
4708.6318	4708.6299	0.0019	3	1	3	4	3	2	1	2	3	3
4777.0262	4777.0288	-0.0026	3	0	3	4	4	2	0	2	3	3
4776.9529	4776.9485	0.0044	3	0	3	3	3	2	0	2	2	2
4776.8135	4776.8127	0.0008	3	0	3	3	3	2	0	2	3	3
4777.1909	4777.1858	0.0051	3	0	3	3	2	2	0	2	2	1
5694.0954	5694.0938	0.0016	3	2	2	4	4	2	2	1	3	3
5694.0954	5694.0938	0.0016	3	2	2	3	4	2	2	1	3	3
5694.3107	5694.3123	-0.0016	3	2	2	2	3	2	2	1	1	2
5693.9158	5693.9172	-0.0014	3	2	2	3	4	2	2	1	2	3
5693.9158	5693.9173	-0.0015	3	2	2	4	4	2	2	1	2	3
5693.9158	5693.9173	-0.0015	3	2	2	3	3	2	2	1	2	3
5693.8548	5693.8572	-0.0024	3	2	2	3	3	2	2	1	2	2
6091.6782	6091.6895	-0.0113	4	1	4	5	5	3	1	3	4	4
6091.6782	6091.6889	-0.0107	4	1	4	3	3	3	1	3	2	2
6106.3305	6106.3347	-0.0042	4	0	4	5	5	3	0	3	4	4
6106.4757	6106.4905	-0.0148	4	0	4	5	6	3	0	3	4	5
6160.6772	6160.6739	0.0033	3	1	2	4	3	2	1	1	3	2
6160.4341	6160.4348	-0.0007	3	1	2	4	5	2	1	1	3	4
6160.1007	6160.1101	-0.0094	3	1	2	4	4	2	1	1	3	3

6610.8093	6610.8061	0.0032	3	2	1	3	4	2	2	0	2	3
6610.9812	6610.9889	-0.0077	3	2	1	4	5	2	2	0	3	4
7298.5247	7298.5216	0.0031	4	2	3	4	4	3	2	2	3	3
7298.6109	7298.6092	0.0017	4	2	3	5	5	3	2	2	4	4
7298.7987	7298.8068	-0.0081	4	2	3	5	6	3	2	2	4	5
7454.4414	7454.4251	0.0163	5	1	5	6	7	4	1	4	5	6
7454.3231	7454.3271	-0.004	5	1	5	6	6	4	1	4	5	5
7456.806	7456.7996	0.0064	5	0	5	6	6	4	0	4	5	5
7456.9258	7456.9007	0.0251	5	0	5	6	7	4	0	4	5	6
7576.4887	7576.4821	0.0066	4	1	3	5	5	3	1	2	4	4
7576.419	7576.4186	0.0004	4	1	3	4	4	3	1	2	3	3
7576.9884	7576.9984	-0.01	4	1	3	5	4	3	1	2	4	3
7576.8593	7576.8618	-0.0025	4	1	3	5	6	3	1	2	4	5
2185.708	2185.7048	0.0032	1	1	1	1	1	0	0	0	1	2
4777.2926	4777.3007	-0.0081	3	0	3	4	3	2	0	2	3	2
3076.4583	3076.4576	0.0007	3	1	2	3	3	3	1	3	3	3
6091.8187	6091.8166	0.0021	4	1	4	3	4	3	1	3	2	3

Table S16: List of lines assigned for the C5 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2752.3817	2752.3766	0.0051	4	2	2	5	4	4	2	3	5	4
3276.4968	3276.4957	0.0011	2	1	2	3	4	1	1	1	2	3
3276.5886	3276.5821	0.0065	2	1	2	1	2	1	1	1	0	1
3467.6829	3467.678	0.0049	2	0	2	3	4	1	0	1	2	3
3467.5576	3467.5479	0.0097	2	0	2	2	3	1	0	1	2	2
3467.4135	3467.4116	0.0019	2	0	2	1	2	1	0	1	0	1
3480.3795	3480.3752	0.0043	3	2	2	4	5	3	0	3	4	5
4378.712	4378.7126	-0.0006	2	1	1	3	4	1	1	0	2	3
4378.8289	4378.8233	0.0056	2	1	1	1	2	1	1	0	0	1
4378.5281	4378.5353	-0.0072	2	1	1	2	3	1	1	0	1	2
4597.8857	4597.895	-0.0093	4	1	3	5	6	4	1	4	5	6
4730.3561	4730.3516	0.0045	3	1	3	4	5	2	1	2	3	4
4730.2817	4730.2778	0.0039	3	1	3	3	4	2	1	2	2	3
4730.1741	4730.1732	0.0009	3	1	3	4	4	2	1	2	3	3
4730.08	4730.078	0.002	3	1	3	3	3	2	1	2	2	2
4729.9724	4729.9768	-0.0044	3	1	3	3	3	2	1	2	3	3
4729.4094	4729.402	0.0074	3	1	3	4	4	2	1	2	3	4
4791.9187	4791.9188	-0.0001	3	0	3	3	3	2	0	2	2	2
4791.9864	4791.9917	-0.0053	3	0	3	4	4	2	0	2	3	3

4792.1571	4792.1542	0.0029	3	0	3	3	2	2	0	2	2	1
4806.5105	4806.5096	0.0009	3	1	3	4	5	2	0	2	3	4
4806.2071	4806.2066	0.0005	3	1	3	4	4	2	0	2	3	3
4806.1345	4806.1388	-0.0043	3	1	3	3	3	2	0	2	2	2
6117.2597	6117.2765	-0.0168	4	1	4	5	6	3	1	3	4	5
6117.1253	6117.1401	-0.0148	4	1	4	5	5	3	1	3	4	4
6115.0729	6115.0856	-0.0127	4	0	4	5	6	3	1	3	4	5
6114.9376	6114.9521	-0.0145	4	0	4	5	5	3	1	3	4	4
6114.9376	6114.9514	-0.0138	4	0	4	3	3	3	1	3	2	2
6129.2925	6129.2869	0.0056	4	0	4	4	5	3	0	3	3	4
6129.1761	6129.167	0.0091	4	0	4	5	5	3	0	3	4	4
6129.1761	6129.1651	0.011	4	0	4	3	3	3	0	3	2	2
6195.6981	6195.7046	-0.0065	3	1	2	4	4	2	1	1	3	3
6196.0483	6196.0482	0.0001	3	1	2	4	5	2	1	1	3	4
6690.2309	6690.2242	0.0067	3	2	1	3	4	2	2	0	2	3
7343.6203	7343.6301	-0.0098	4	2	3	5	6	3	2	2	4	5
7343.5535	7343.5383	0.0152	4	2	3	4	5	3	2	2	3	4
7343.4375	7343.4271	0.0104	4	2	3	5	5	3	2	2	4	4
7343.3555	7343.3427	0.0128	4	2	3	4	4	3	2	2	3	3
7484.2691	7484.2786	-0.0095	5	1	5	6	6	4	1	4	5	5
7484.3862	7484.3773	0.0089	5	1	5	6	7	4	1	4	5	6
7486.1586	7486.1628	-0.0042	5	0	5	6	6	4	0	4	5	5
7486.2784	7486.2642	0.0142	5	0	5	6	7	4	0	4	5	6
7595.891	7595.8914	-0.0004	4	1	3	4	4	3	1	2	3	3
7595.9488	7595.9545	-0.0057	4	1	3	5	5	3	1	2	4	4
7596.339	7596.332	0.007	4	1	3	5	6	3	1	2	4	5
7596.4668	7596.4683	-0.0015	4	1	3	5	4	3	1	2	4	3
2752.6303	2752.6329	-0.0026	4	2	2	4	5	4	2	3	4	5
2753.5076	2753.51	-0.0024	4	2	2	4	4	4	2	3	4	4
3275.7271	3275.7245	0.0026	2	1	2	3	3	1	1	1	2	3
3467.0902	3467.0975	-0.0073	2	0	2	3	3	1	0	1	2	2
3480.0824	3480.0738	0.0086	3	2	2	4	3	3	0	3	4	3
3481.3047	3481.3033	0.0014	3	2	2	4	4	3	0	3	4	4
3481.5131	3481.5047	0.0084	3	2	2	3	3	3	0	3	3	3
3962.0715	3962.0787	-0.0072	5	4	2	5	6	5	3	3	5	6
3961.9254	3961.9185	0.0069	5	4	2	6	7	5	3	3	6	7
4695.5545	4695.5634	-0.0089	4	2	3	5	5	4	0	4	5	5
4694.6762	4694.6832	-0.007	4	2	3	5	6	4	0	4	5	6
4716.1169	4716.1152	0.0017	3	0	3	4	5	2	1	2	3	4
4716.0206	4716.0357	-0.0151	3	0	3	3	4	2	1	2	2	3
5741.1074	5741.1116	-0.0042	3	2	2	3	4	2	2	1	2	3
5741.3791	5741.3797	-0.0006	3	2	2	4	5	2	2	1	3	4

5741.5139	5741.5084	0.0055	3	2	2	2	3	2	2	1	1	2
6196.3007	6196.2974	0.0033	3	1	2	4	3	2	1	1	3	2
6690.6073	6690.608	-0.0007	3	2	1	2	2	2	2	0	1	1
6690.6073	6690.6058	0.0015	3	2	1	2	1	2	2	0	1	0
6690.4126	6690.4166	-0.004	3	2	1	4	5	2	2	0	3	4
3276.2961	3276.2908	0.0053	2	1	2	2	3	1	1	1	1	2
4792.2709	4792.2731	-0.0022	3	0	3	4	5	2	0	2	3	4

Table S17: List of lines assigned for the C6 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2286.282	2286.2805	0.0015	5	3	2	6	6	5	3	3	6	6
3227.6644	3227.6685	-0.0041	3	3	1	4	5	3	1	2	4	5
3227.5431	3227.5399	0.0032	3	3	1	2	3	3	1	2	2	3
3294.2525	3294.2532	-0.0007	2	1	2	3	4	1	1	1	2	3
3294.3398	3294.3414	-0.0016	2	1	2	1	2	1	1	1	0	1
3294.0435	3294.045	-0.0015	2	1	2	2	3	1	1	1	1	2
3293.4824	3293.4833	-0.0009	2	1	2	3	3	1	1	1	2	3
3293.7638	3293.769	-0.0052	2	1	2	3	2	1	1	1	1	1
3293.9648	3293.969	-0.0042	2	1	2	2	2	1	1	1	2	1
3293.3442	3293.3373	0.0069	2	1	2	2	2	1	1	1	1	2
3483.7066	3483.7045	0.0021	2	0	2	3	4	1	0	1	2	3
3491.3493	3491.3515	-0.0022	3	2	2	4	5	3	0	3	4	5
3491.6078	3491.6033	0.0045	3	2	2	3	4	3	0	3	3	4
3491.0535	3491.0507	0.0028	3	2	2	4	3	3	0	3	4	3
3492.2868	3492.2812	0.0056	3	2	2	4	4	3	0	3	4	4
3492.2198	3492.2167	0.0031	3	2	2	2	2	3	0	3	2	2
3490.9441	3490.938	0.0061	3	2	2	2	1	3	0	3	2	1
3490.9441	3490.938	0.0061	3	2	2	3	2	3	0	3	2	1
3492.4857	3492.4928	-0.0071	3	2	2	3	3	3	0	3	3	3
4624.4758	4624.4843	-0.0085	4	1	3	5	6	4	1	4	5	6
4753.7715	4753.7665	0.005	3	1	3	4	5	2	1	2	3	4
4753.6934	4753.6894	0.004	3	1	3	3	4	2	1	2	2	3
4753.4924	4753.4875	0.0049	3	1	3	3	3	2	1	2	2	2
4752.8126	4752.8172	-0.0046	3	1	3	4	4	2	1	2	3	4
4752.8126	4752.811	0.0016	3	1	3	2	2	2	1	2	1	2
4753.8811	4753.8768	0.0043	3	1	3	2	1	2	1	2	2	1
4753.3754	4753.3801	-0.0047	3	1	3	3	3	2	1	2	3	3
4754.7523	4754.7522	0.0001	3	1	3	3	2	2	1	2	2	2
4754.847	4754.8446	0.0024	3	1	3	4	3	2	1	2	3	3

4753.5924	4753.587	0.0054	3	1	3	4	4	2	1	2	3	3
4813.4897	4813.4951	-0.0054	3	0	3	4	4	2	0	2	3	3
4813.4223	4813.4169	0.0054	3	0	3	3	3	2	0	2	2	2
4813.6433	4813.6413	0.002	3	0	3	3	2	2	0	2	2	1
4813.7447	4813.7542	-0.0095	3	0	3	2	3	2	0	2	1	2
4813.9616	4813.9577	0.0039	3	0	3	2	1	2	0	2	2	1
4814.0576	4814.0458	0.0118	3	0	3	2	3	2	0	2	2	3
4813.2887	4813.2835	0.0052	3	0	3	3	3	2	0	2	3	3
4814.6568	4814.6555	0.0013	3	0	3	3	2	2	0	2	2	2
4814.7262	4814.7257	0.0005	3	0	3	4	3	2	0	2	3	3
5775.0384	5775.0356	0.0028	3	2	2	3	4	2	2	1	2	3
5774.9706	5774.9679	0.0027	3	2	2	3	3	2	2	1	2	2
5775.2131	5775.2097	0.0034	3	2	2	4	4	2	2	1	3	3
6146.4411	6146.4529	-0.0118	4	1	4	5	6	3	1	3	4	5
6146.313	6146.3176	-0.0046	4	1	4	5	5	3	1	3	4	4
6146.313	6146.3169	-0.0039	4	1	4	3	3	3	1	3	2	2
6157.8558	6157.866	-0.0102	4	0	4	5	6	3	0	3	4	5
6157.8558	6157.8573	-0.0015	4	0	4	3	4	3	0	3	2	3
6157.7179	6157.7137	0.0042	4	0	4	5	5	3	0	3	4	4
6157.7179	6157.7121	0.0058	4	0	4	3	3	3	0	3	2	2
6227.6535	6227.6649	-0.0114	3	1	2	4	4	2	1	1	3	3
6228.0028	6228.0094	-0.0066	3	1	2	4	5	2	1	1	3	4
6228.0028	6228.0124	-0.0096	3	1	2	2	3	2	1	1	1	2
6228.2432	6228.254	-0.0108	3	1	2	4	3	2	1	1	3	2
6379.9889	6379.9904	-0.0015	2	2	0	3	4	1	0	1	2	3
7382.2237	7382.2201	0.0036	4	2	3	4	4	3	2	2	3	3
7382.3039	7382.307	-0.0031	4	2	3	5	5	3	2	2	4	4
7382.431	7382.4198	0.0112	4	2	3	4	5	3	2	2	3	4
7519.7695	7519.762	0.0075	5	1	5	6	7	4	1	4	5	6
7519.6556	7519.6643	-0.0087	5	1	5	6	6	4	1	4	5	5
7521.5188	7521.5115	0.0073	5	0	5	6	7	4	0	4	5	6
7521.408	7521.4115	-0.0035	5	0	5	6	6	4	0	4	5	5
5775.4415	5775.4407	0.0008	3	2	2	2	3	2	2	1	1	2
5775.5283	5775.5196	0.0087	3	2	2	2	1	2	2	1	1	0

Table S18: List of lines assigned for the N11 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs- Calc [MHz]	J'	K'_a	K'_c	F'	J	K_a	K_c	F
2533.9141	2533.9154	-0.0013	2	2	1	3	2	0	2	3
2533.5282	2533.53	-0.0018	2	2	1	1	2	0	2	1

2534.612	2534.6097	0.0023	2	2	1	2	2	0	2	2
3126.2533	3126.2546	-0.0013	3	1	2	4	3	1	3	4
3473.8697	3473.8662	0.0035	2	0	2	2	1	0	1	1
3473.7762	3473.7778	-0.0016	2	0	2	2	1	0	1	2
3474.3791	3474.3773	0.0018	2	0	2	3	1	0	1	2
3474.5838	3474.5778	0.006	2	0	2	1	1	0	1	0
3474.7994	3474.7989	0.0005	2	0	2	1	1	0	1	1
4387.2769	4387.2764	0.0005	2	1	1	1	1	1	0	1
4703.5397	4703.5396	0.0001	4	2	3	5	4	0	4	5
4703.3195	4703.3165	0.003	4	2	3	3	4	0	4	3
4704.4073	4704.4073	0	4	2	3	4	4	0	4	4
4739.5845	4739.5851	-0.0006	3	1	3	3	2	1	2	2
4739.6748	4739.6774	-0.0026	3	1	3	2	2	1	2	1
4739.7648	4739.7661	-0.0013	3	1	3	4	2	1	2	3
4740.8238	4740.8281	-0.0043	3	1	3	2	2	1	2	2
4738.8436	4738.8454	-0.0018	3	1	3	3	2	1	2	3
4800.5366	4800.5405	-0.0039	3	0	3	3	2	0	2	3
4801.1408	4801.1401	0.0007	3	0	3	3	2	0	2	2
4801.4457	4801.4383	0.0074	3	0	3	4	2	0	2	3
4802.3529	4802.3522	0.0007	3	0	3	2	2	0	2	2
5753.6662	5753.6602	0.006	3	2	2	4	2	2	1	3
5753.5647	5753.5655	-0.0008	3	2	2	3	2	2	1	2
6129.2916	6129.2833	0.0083	4	1	4	5	3	1	3	4
6141.2243	6141.2344	-0.0101	4	0	4	5	3	0	3	4
6141.0759	6141.0733	0.0026	4	0	4	4	3	0	3	3
6705.8648	6705.8589	0.0059	3	2	1	4	2	2	0	3
6706.0536	6706.059	-0.0054	3	2	1	3	2	2	0	2
7358.4515	7358.4453	0.0062	4	2	3	4	3	2	2	3
7499.0172	7499.0182	-0.001	5	1	5	6	4	1	4	5
7498.921	7498.916	0.005	5	1	5	5	4	1	4	4
7500.7805	7500.7785	0.002	5	0	5	5	4	0	4	4
7500.8791	7500.8833	-0.0042	5	0	5	6	4	0	4	5
7610.1717	7610.1763	-0.0046	4	1	3	4	3	1	2	3
7610.7043	7610.708	-0.0037	4	1	3	3	3	1	2	2
7610.573	7610.5772	-0.0042	4	1	3	5	3	1	2	4
4388.3236	4388.3249	-0.0013	2	1	1	3	1	1	0	2
4388.9979	4389.0022	-0.0043	2	1	1	1	1	1	0	0
2761.9332	2761.9319	0.0013	4	2	2	4	4	2	3	4
2761.0547	2761.0554	-0.0007	4	2	2	5	4	2	3	5
2760.8283	2760.8299	-0.0016	4	2	2	3	4	2	3	3
6208.5576	6208.5526	0.005	3	1	2	4	2	1	1	3
6208.2119	6208.2064	0.0055	3	1	2	3	2	1	1	2

6208.808	6208.8063	0.0017	3	1	2	2	2	1	1	1
7358.6342	7358.6366	-0.0024	4	2	3	5	3	2	2	4
3282.4912	3282.4942	-0.003	2	1	2	2	1	1	1	2
3282.7369	3282.7418	-0.0049	2	1	2	1	1	1	1	0
3283.0935	3283.0962	-0.0027	2	1	2	2	1	1	1	1
3283.2322	3283.2339	-0.0017	2	1	2	3	1	1	1	2
3127.4701	3127.474	-0.0039	3	1	2	3	3	1	3	3

Table S19: List of lines assigned for the O12 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
3239.2872	3239.2878	-0.0006	2	1	2	3	4	1	1	1	2	3
3441.6028	3441.5986	0.0042	2	0	2	3	4	1	0	1	2	3
3441.4628	3441.4596	0.0032	2	0	2	2	3	1	0	1	2	2
3440.9668	3440.9679	-0.0011	2	0	2	3	3	1	0	1	2	3
4308.6918	4308.6929	-0.0011	2	1	1	1	2	1	1	0	0	1
4308.3997	4308.3992	0.0005	2	1	1	2	3	1	1	0	1	2
4687.8697	4687.8731	-0.0034	3	1	3	4	5	2	1	2	3	4
4687.8697	4687.8743	-0.0046	3	1	3	2	3	2	1	2	1	2
4687.7895	4687.7947	-0.0052	3	1	3	3	4	2	1	2	2	3
5660.8719	5660.8731	-0.0012	3	2	2	4	5	2	2	1	3	4
5660.6046	5660.5996	0.005	3	2	2	3	4	2	2	1	2	3
5660.5377	5660.5386	-0.0009	3	2	2	3	3	2	2	1	2	2
5660.7855	5660.781	0.0045	3	2	2	4	4	2	2	1	3	3
5660.7855	5660.781	0.0045	3	2	2	3	4	2	2	1	3	3
5661.0024	5661.0044	-0.002	3	2	2	2	3	2	2	1	1	2
6068.2348	6068.2352	-0.0004	4	1	4	5	5	3	1	3	4	4
6084.2837	6084.2829	0.0008	4	0	4	5	6	3	0	3	4	5
6560.6215	6560.6188	0.0027	3	2	1	4	5	2	2	0	3	4
7426.3469	7426.3521	-0.0052	5	1	5	6	6	4	1	4	5	5
7429.231	7429.2247	0.0063	5	0	5	6	7	4	0	4	5	6
7429.1205	7429.1231	-0.0026	5	0	5	6	6	4	0	4	5	5
7551.5686	7551.5721	-0.0035	4	1	3	5	6	3	1	2	4	5
7551.7046	7551.7102	-0.0056	4	1	3	5	4	3	1	2	4	3
7551.1955	7551.1925	0.003	4	1	3	5	5	3	1	2	4	4
7551.1368	7551.1312	0.0056	4	1	3	4	4	3	1	2	3	3
4308.5739	4308.5769	-0.003	2	1	1	3	4	1	1	0	2	3
4308.3365	4308.3389	-0.0024	2	1	1	1	1	1	1	0	1	0
6068.3691	6068.3693	-0.0002	4	1	4	5	6	3	1	3	4	5
4307.4708	4307.4726	-0.0018	2	1	1	3	2	1	1	0	2	2

3441.2428	3441.2414	0.0014	2	0	2	3	3	1	0	1	1	2
3441.8453	3441.8434	0.0019	2	0	2	3	2	1	0	1	2	1
3240.2517	3240.2506	0.0011	2	1	2	3	2	1	1	1	2	2
3240.1693	3240.1684	0.0009	2	1	2	2	1	1	1	1	2	2
3239.3775	3239.3767	0.0008	2	1	2	1	2	1	1	1	0	1
7426.45	7426.4502	-0.0002	5	1	5	6	7	4	1	4	5	6
6084.1341	6084.126	0.0081	4	0	4	5	5	3	0	3	4	4
3441.3291	3441.331	-0.0019	2	0	2	1	2	1	0	1	2	1
7262.9644	7262.9681	-0.0037	4	2	3	1	5	3	2	2	1	4
4247.2052	4247.2088	-0.0036	5	2	3	1	6	5	2	4	1	6
4247.1346	4247.1315	0.0031	5	2	3	2	7	5	2	4	2	7
3239.075	3239.0781	-0.0031	2	1	2	1	3	1	1	1	1	2
3239.0125	3239.0142	-0.0017	2	1	2	0	2	1	1	1	2	1

Table S20: List of lines assigned for the O13 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
4671.3177	4671.3227	-0.005	3	1	3	3	4	2	1	2	2	3
4671.2053	4671.2115	-0.0062	3	1	3	4	4	2	1	2	3	3
4671.4998	4671.4978	0.002	3	1	3	2	1	2	1	2	2	1
4724.2514	4724.2526	-0.0012	3	0	3	4	5	2	0	2	3	4
4724.1318	4724.1328	-0.001	3	0	3	3	2	2	0	2	2	1
5690.8839	5690.8835	0.0004	3	2	2	4	5	2	2	1	3	4
6036.7856	6036.783	0.0026	4	1	4	5	5	3	1	3	4	4
6036.7342	6036.7287	0.0055	4	1	4	4	4	3	1	3	3	3
6046.1645	6046.1685	-0.004	4	0	4	5	5	3	0	3	4	4
6122.6155	6122.6207	-0.0052	3	1	2	4	4	2	1	1	3	3
6123.0146	6123.017	-0.0024	3	1	2	4	5	2	1	1	3	4
6657.459	6657.4535	0.0055	3	2	1	4	5	2	2	0	3	4
6657.2581	6657.2572	0.0009	3	2	1	3	4	2	2	0	2	3
7386.2119	7386.2147	-0.0028	5	0	5	6	6	4	0	4	5	5
7386.2119	7386.2098	0.0021	5	0	5	4	4	4	0	4	3	3
7386.3285	7386.3217	0.0068	5	0	5	6	7	4	0	4	5	6
7482.0583	7482.0487	0.0096	4	1	3	5	5	3	1	2	4	4
7482.5182	7482.5131	0.0051	4	1	3	5	6	3	1	2	4	5
7261.5158	7261.5246	-0.0088	4	2	3	5	6	3	2	2	4	5
4346.1094	4346.1168	-0.0074	2	1	1	2	3	1	1	0	1	2
4345.0977	4345.0986	-0.0009	2	1	1	3	2	1	1	0	2	2
6046.3296	6046.3321	-0.0025	4	0	4	5	6	3	0	3	4	5
6036.917	6036.928	-0.011	4	1	4	5	6	3	1	3	4	5

4346.2955	4346.2984	-0.0029	2	1	1	3	4	1	1	0	2	3
7482.6596	7482.6619	-0.0023	4	1	3	5	4	3	1	2	4	3
7384.8654	7384.8654	0	5	1	5	6	6	4	1	4	5	5
7384.925	7384.9208	0.0042	5	1	5	4	3	4	1	4	3	2
7384.9732	7384.9701	0.0031	5	1	5	6	7	4	1	4	5	6
3419.9672	3419.9686	-0.0014	2	0	2	3	4	1	0	1	2	3
3419.333	3419.3334	-0.0004	2	0	2	3	3	1	0	1	2	2
4724.2033	4724.2066	-0.0033	3	0	3	3	4	2	0	2	2	3
4346.4098	4346.4119	-0.0021	2	1	1	1	2	1	1	0	0	1
3419.7033	3419.7014	0.0019	2	0	2	1	2	1	0	1	0	1
3420.2698	3420.2688	0.001	2	0	2	3	2	1	0	1	2	1
6657.673	6657.67	0.003	3	2	1	4	4	2	2	0	3	3
6657.5418	6657.5388	0.003	3	2	1	2	3	2	2	0	1	2
4671.4016	4671.398	0.0036	3	1	3	2	5	2	1	2	2	4

Table S21: List of lines assigned for the C14 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
3144.8327	3144.8383	-0.0056	3	1	2	3	3	3	1	3	3	3
3143.6725	3143.671	0.0015	3	1	2	3	4	3	1	3	3	4
3143.5155	3143.5122	0.0033	3	1	2	4	5	3	1	3	4	5
3143.4537	3143.4583	-0.0046	3	1	2	2	3	3	1	3	2	3
3467.9554	3467.9567	-0.0013	2	0	2	3	4	1	0	1	2	3
3467.8503	3467.846	0.0043	2	0	2	2	3	1	0	1	2	2
3468.1994	3468.1992	0.0002	2	0	2	3	2	1	0	1	2	1
3468.0415	3468.0442	-0.0027	2	0	2	2	3	1	0	1	1	2
3467.6829	3467.6821	0.0008	2	0	2	1	2	1	0	1	0	1
4399.4238	4399.4299	-0.0061	2	1	1	3	4	1	1	0	2	3
4399.5395	4399.5415	-0.002	2	1	1	1	2	1	1	0	0	1
4398.3605	4398.3552	0.0053	2	1	1	3	2	1	1	0	2	2
4735.0629	4735.0676	-0.0047	3	1	3	4	5	2	1	2	3	4
4734.9874	4734.9918	-0.0044	3	1	3	3	4	2	1	2	2	3
4734.7792	4734.7852	-0.006	3	1	3	3	3	2	1	2	2	2
4734.6698	4734.6778	-0.008	3	1	3	3	3	2	1	2	3	3
4735.1773	4735.1793	-0.002	3	1	3	2	1	2	1	2	2	1
4735.3048	4735.3075	-0.0027	3	1	3	2	3	2	1	2	2	3
4736.0462	4736.0543	-0.0081	3	1	3	3	2	2	1	2	2	2
4736.1398	4736.1457	-0.0059	3	1	3	4	3	2	1	2	3	3
4734.1073	4734.115	-0.0077	3	1	3	4	4	2	1	2	3	4
4790.9244	4790.92	0.0044	3	0	3	3	4	2	0	2	2	3

4790.8341	4790.8347	-0.0006	3	0	3	3	2	2	0	2	2	1
4791.1503	4791.1487	0.0016	3	0	3	2	1	2	0	2	2	1
4790.7036	4790.7046	-0.001	3	0	3	4	4	2	0	2	3	3
4790.6299	4790.6252	0.0047	3	0	3	3	3	2	0	2	2	2
4790.4974	4790.4948	0.0026	3	0	3	3	3	2	0	2	3	3
4791.2454	4791.2415	0.0039	3	0	3	2	3	2	0	2	2	3
6120.1767	6120.1896	-0.0129	4	1	4	5	5	3	1	3	4	4
6120.1767	6120.1889	-0.0122	4	1	4	3	3	3	1	3	2	2
6130.3748	6130.3816	-0.0068	4	0	4	5	5	3	0	3	4	4
6205.9749	6205.9716	0.0033	3	1	2	4	3	2	1	1	3	2
6205.733	6205.7362	-0.0032	3	1	2	4	5	2	1	1	3	4
6205.3928	6205.3915	0.0013	3	1	2	4	4	2	1	1	3	3
7357.9716	7357.967	0.0046	4	2	3	4	5	3	2	2	3	4
7358.065	7358.059	0.006	4	2	3	5	6	3	2	2	4	5
7357.8334	7357.8419	-0.0085	4	2	3	5	5	3	2	2	4	4
7357.7672	7357.7574	0.0098	4	2	3	4	4	3	2	2	3	3
7358.1582	7358.1385	0.0197	4	2	3	3	2	3	2	2	2	1
7487.2667	7487.2537	0.013	5	1	5	6	7	4	1	4	5	6
7487.1584	7487.1568	0.0016	5	1	5	6	6	4	1	4	5	5
7488.7691	7488.7575	0.0116	5	0	5	6	7	4	0	4	5	6
7488.6561	7488.6589	-0.0028	5	0	5	6	6	4	0	4	5	5
7488.6561	7488.6541	0.002	5	0	5	4	4	4	0	4	3	3
7590.3766	7590.368	0.0086	4	1	3	5	4	3	1	2	4	3
7590.2563	7590.241	0.0153	4	1	3	5	6	3	1	2	4	5
7589.8187	7589.8172	0.0015	4	1	3	4	4	3	1	2	3	3
3696.2372	3696.2418	-0.0046	4	3	2	5	4	4	1	3	5	4
3696.177	3696.1816	-0.0046	4	3	2	3	2	4	1	3	3	2
3467.4132	3467.4137	-0.0005	2	0	2	2	2	1	0	1	1	1
3467.566	3467.5728	-0.0068	2	0	2	3	3	1	0	1	1	2
3467.2798	3467.2857	-0.0059	2	0	2	3	3	1	0	1	2	3
3144.6932	3144.6932	0	3	1	2	4	4	3	1	3	4	4
3283.6513	3283.6545	-0.0032	2	1	2	3	2	1	1	1	1	1
3283.5716	3283.5727	-0.0011	2	1	2	2	1	1	1	1	1	1
3283.756	3283.7569	-0.0009	2	1	2	2	2	1	1	1	2	1
3284.1652	3284.1657	-0.0005	2	1	2	1	2	1	1	1	0	1
4399.2566	4399.264	-0.0074	2	1	1	2	3	1	1	0	1	2
3284.0819	3284.0812	0.0007	2	1	2	3	4	1	1	1	2	3
6130.5229	6130.5307	-0.0078	4	0	4	2	6	3	0	3	2	5
6120.3132	6120.3246	-0.0114	4	1	4	2	6	3	1	3	2	5

Table S22: List of lines assigned for the N15 isotopologue of 2-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	F'	J	K_a	K_c	F
3263.4921	3263.4903	0.0018	2	1	2	3	1	1	1	2
3263.5616	3263.565	-0.0034	2	1	2	1	1	1	1	1
3263.6538	3263.6531	0.0007	2	1	2	1	1	1	1	0
3432.4069	3432.4056	0.0013	3	2	2	3	3	0	3	3
3432.1348	3432.1339	0.0009	3	2	2	4	3	0	3	4
3432.0412	3432.0389	0.0023	3	2	2	2	3	0	3	2
3440.5312	3440.5267	0.0045	2	0	2	3	1	0	1	2
3440.879	3440.8774	0.0016	2	0	2	1	1	0	1	1
4379.3334	4379.3266	0.0068	2	1	1	2	1	1	0	1
4379.5448	4379.549	-0.0042	2	1	1	3	1	1	0	2
4379.8471	4379.8471	0	2	1	1	1	1	1	0	0
4700.6365	4700.6394	-0.0029	3	1	3	3	2	1	2	3
4700.8364	4700.8372	-0.0008	3	1	3	3	2	1	2	2
4700.9114	4700.9064	0.005	3	1	3	4	2	1	2	3
4701.1994	4701.1978	0.0016	3	1	3	2	2	1	2	2
4751.9728	4751.9722	0.0006	3	0	3	3	2	0	2	3
5732.0265	5732.0249	0.0016	3	2	2	3	2	2	1	2
5732.2572	5732.2605	-0.0033	3	2	2	4	2	2	1	3
5732.3872	5732.3915	-0.0043	3	2	2	2	2	2	1	1
6074.0912	6074.095	-0.0038	4	1	4	5	3	1	3	4
6074.0912	6074.0796	0.0116	4	1	4	3	3	1	3	2
6712.0254	6712.0234	0.002	3	2	1	3	2	2	0	2
6712.2341	6712.2315	0.0026	3	2	1	4	2	2	0	3
6712.3537	6712.3527	0.001	3	2	1	2	2	2	0	1
7309.9132	7309.9039	0.0093	4	2	3	4	3	2	2	3
7309.9933	7310.0014	-0.0081	4	2	3	5	3	2	2	4
7430.1643	7430.1625	0.0018	5	1	5	6	4	1	4	5
7431.4173	7431.4215	-0.0042	5	0	5	6	4	0	4	5
7525.8476	7525.8601	-0.0125	4	1	3	5	3	1	2	4
3638.939	3638.9343	0.0047	4	3	2	4	4	1	3	4
3440.3217	3440.3276	-0.0059	2	0	2	1	1	0	1	0
4752.2444	4752.2438	0.0006	3	0	3	4	2	0	2	3
4659.0881	4659.0987	-0.0106	4	2	3	5	4	0	4	5
4690.4473	4690.4521	-0.0048	3	0	3	3	2	1	2	2
4690.5252	4690.5259	-0.0007	3	0	3	4	2	1	2	3
6163.0516	6163.0441	0.0075	3	1	2	4	2	1	1	3
3263.2596	3263.2572	0.0024	2	1	2	2	1	1	1	1
2452.1165	2452.1172	-0.0007	2	2	1	3	2	0	2	3

3136.1421	3136.1433	-0.0012	3	1	2	2	3	1	3	2
3136.2087	3136.207	0.0017	3	1	2	4	3	1	3	4
3638.675	3638.6711	0.0039	4	3	2	3	4	1	3	3
2451.8548	2451.8556	-0.0008	2	2	1	1	2	0	2	1
3638.725	3638.725	0	4	3	2	5	4	1	3	5

Table S23: List of lines assigned for the parent isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2239.874	2239.87	0.004	3	1	2	3	4	3	0	3	3	4
2240.3812	2240.3769	0.0043	3	1	2	3	3	3	0	3	3	3
2344.6138	2344.6147	-0.0009	9	2	8	9	10	8	3	5	8	9
2380.9512	2380.9525	-0.0013	7	2	5	8	8	6	3	4	7	7
2528.4421	2528.4453	-0.0032	3	0	3	3	2	2	1	2	2	1
2528.2799	2528.279	0.0009	3	0	3	3	3	2	1	2	2	2
2730.5469	2730.5515	-0.0046	4	1	3	5	6	4	0	4	5	6
2730.7567	2730.7526	0.0041	4	1	3	4	5	4	0	4	4	5
2731.0364	2731.0403	-0.0039	4	1	3	5	5	4	0	4	5	5
2731.2292	2731.2242	0.005	4	1	3	4	4	4	0	4	4	4
2833.8977	2833.895	0.0027	1	1	1	2	3	0	0	0	1	2
2833.677	2833.6713	0.0057	1	1	1	1	1	0	0	0	1	2
2833.677	2833.6712	0.0058	1	1	1	1	1	0	0	0	1	1
3962.0706	3962.0691	0.0015	2	1	2	3	3	1	0	1	2	2
3977.3819	3977.3836	-0.0017	4	0	4	5	6	3	1	3	4	5
3977.325	3977.3268	-0.0018	4	0	4	5	4	3	1	3	4	3
4030.5612	4030.5553	0.0059	6	2	4	7	7	6	1	5	7	7
4030.3756	4030.3733	0.0023	6	2	4	5	6	6	1	5	5	6
5979.1171	5979.1181	-0.001	4	1	4	5	6	3	0	3	4	5
5979.1171	5979.1193	-0.0022	4	1	4	3	4	3	0	3	2	3
7373.847	7373.8453	0.0017	2	2	1	3	3	1	1	0	2	2
7374.0387	7374.0349	0.0038	2	2	1	2	2	1	1	0	1	1
7374.1668	7374.1668	0	2	2	1	3	2	1	1	0	2	1
7575.591	7575.5929	-0.0019	2	2	0	3	4	1	1	1	2	3
7575.8029	7575.8075	-0.0046	2	2	0	2	3	1	1	1	1	2
7575.5075	7575.5031	0.0044	2	2	0	1	2	1	1	1	2	1
7575.374	7575.38	-0.006	2	2	0	3	2	1	1	1	1	1
6707.1335	6707.1321	0.0014	8	3	5	9	10	8	2	6	9	10
6707.1335	6707.133	0.0005	8	3	5	7	8	8	2	6	7	8
6707.1962	6707.1978	-0.0016	8	3	5	9	9	8	2	6	9	9
6707.1962	6707.1987	-0.0025	8	3	5	7	7	8	2	6	7	7

6919.9728	6919.9664	0.0064	5	1	5	5	5	4	0	4	4	4
5003.3536	5003.3572	-0.0036	3	1	3	2	3	2	0	2	1	2
4275.5372	4275.5351	0.0021	6	1	5	6	5	6	0	6	6	5
4275.6187	4275.6191	-0.0004	6	1	5	6	7	6	0	6	6	7
4275.879	4275.8792	-0.0002	6	1	5	7	7	6	0	6	7	7
4276.0931	4276.0909	0.0022	6	1	5	6	6	6	0	6	6	6
3406.0532	3406.0542	-0.001	5	1	4	6	7	5	0	5	6	7
3406.741	3406.7339	0.0071	5	1	4	5	5	5	0	5	5	5
3406.5336	3406.5341	-0.0005	5	1	4	6	6	5	0	5	6	6
3406.2723	3406.2656	0.0067	5	1	4	5	6	5	0	5	5	6
3406.1688	3406.163	0.0058	5	1	4	5	4	5	0	5	5	4
3405.9704	3405.9635	0.0069	5	1	4	6	5	5	0	5	6	5
4371.2006	4371.2001	0.0005	3	2	1	3	3	3	1	2	3	3
4371.1331	4371.1304	0.0027	3	2	1	4	4	3	1	2	4	4
4370.6806	4370.6774	0.0032	3	2	1	4	5	3	1	2	4	5
4370.7625	4370.7609	0.0016	3	2	1	3	4	3	1	2	3	4
4575.6167	4575.6212	-0.0045	2	2	0	3	4	2	1	1	3	4
4575.8278	4575.8258	0.002	2	2	0	2	3	2	1	1	2	3
4575.5287	4575.5355	-0.0068	2	2	0	1	2	2	1	1	1	2
4575.0927	4575.0947	-0.002	2	2	0	3	2	2	1	1	3	2
4519.5081	4519.5122	-0.0041	8	2	6	8	8	8	1	7	8	8
4519.4174	4519.4233	-0.0059	8	2	6	9	9	8	1	7	9	9
4519.2122	4519.2108	0.0014	8	2	6	9	10	8	1	7	9	10
5405.8312	5405.8317	-0.0005	3	2	2	4	3	3	1	3	4	3
5406.1286	5406.1262	0.0024	3	2	2	4	5	3	1	3	4	5
5406.4084	5406.4109	-0.0025	3	2	2	3	4	3	1	3	3	4
5407.0493	5407.0466	0.0027	3	2	2	4	4	3	1	3	4	4
5406.974	5406.9749	-0.0009	3	2	2	2	2	3	1	3	2	2
5407.2869	5407.2872	-0.0003	3	2	2	3	3	3	1	3	3	3
5406.0456	5406.043	0.0026	3	2	2	2	3	3	1	3	2	3
5406.0456	5406.043	0.0026	3	2	2	3	3	3	1	3	2	3
5405.7058	5405.7044	0.0014	3	2	2	2	1	3	1	3	2	1
5405.7058	5405.7045	0.0013	3	2	2	3	2	3	1	3	2	1
2240.7239	2240.7279	-0.004	3	1	2	4	3	3	0	3	4	4
2240.6048	2240.5975	0.0073	3	1	2	4	5	3	0	3	4	4
2240.8978	2240.895	0.0028	3	1	2	3	2	3	0	3	3	3
2528.15	2528.1475	0.0025	3	0	3	3	3	2	1	2	3	3
2528.3556	2528.359	-0.0034	3	0	3	4	4	2	1	2	3	3
2528.7599	2528.7614	-0.0015	3	0	3	2	1	2	1	2	2	1
2528.8652	2528.8689	-0.0037	3	0	3	2	3	2	1	2	2	3
2529.5809	2529.5832	-0.0023	3	0	3	4	3	2	1	2	3	3
2529.5083	2529.5111	-0.0028	3	0	3	3	2	2	1	2	2	2

2527.8715	2527.8716	-0.0001	3	0	3	4	4	2	1	2	2	3
2730.3795	2730.3741	0.0054	4	1	3	3	2	4	0	4	3	2
2730.2718	2730.267	0.0048	4	1	3	4	3	4	0	4	3	2
2730.2718	2730.2652	0.0066	4	1	3	4	4	4	0	4	4	5
2730.0625	2730.0554	0.0071	4	1	3	5	5	4	0	4	5	6
2730	2729.9999	0.0001	4	1	3	4	4	4	0	4	4	3
2731.5332	2731.5363	-0.0031	4	1	3	5	6	4	0	4	5	5
2731.6645	2731.6592	0.0053	4	1	3	5	4	4	0	4	5	5
2731.8446	2731.8426	0.002	4	1	3	4	3	4	0	4	4	4
2834.0441	2834.0419	0.0022	1	1	1	2	2	0	0	0	1	2
2834.0441	2834.0418	0.0023	1	1	1	2	2	0	0	0	1	1
2840.8803	2840.8752	0.0051	10	2	9	11	11	9	3	6	10	10
2841.1112	2841.1125	-0.0013	10	2	9	10	11	9	3	6	9	10
3013.293	3013.2865	0.0065	5	1	4	6	6	4	2	3	5	5
3013.293	3013.2864	0.0066	5	1	4	4	4	4	2	3	3	3
3013.4957	3013.4979	-0.0022	5	1	4	6	7	4	2	3	5	6
3013.4957	3013.4965	-0.0008	5	1	4	4	5	4	2	3	3	4
3012.9312	3012.9316	-0.0004	5	1	4	6	6	4	2	3	5	6
3012.9312	3012.9311	0.0001	5	1	4	4	4	4	2	3	3	4
3013.6442	3013.6378	0.0064	5	1	4	4	3	4	2	3	4	3
3013.9683	3013.9645	0.0038	5	1	4	6	5	4	2	3	5	5
3045.4098	3045.4107	-0.0009	11	2	10	10	10	10	3	7	9	9
3045.8235	3045.8257	-0.0022	11	2	10	12	13	10	3	7	11	12
3045.208	3045.2029	0.0051	11	2	10	11	11	10	3	7	10	10
3962.1723	3962.1714	0.0009	2	1	2	1	2	1	0	1	1	2
3962.269	3962.2674	0.0016	2	1	2	1	1	1	0	1	1	0
3963.0975	3963.0962	0.0013	2	1	2	3	2	1	0	1	2	2
3961.1438	3961.1496	-0.0058	2	1	2	3	2	1	0	1	2	1
3961.0587	3961.0569	0.0018	2	1	2	2	1	1	0	1	2	1
3961.2412	3961.2457	-0.0045	2	1	2	3	3	1	0	1	2	3
3961.3074	3961.3063	0.0011	2	1	2	1	0	1	0	1	2	1
3962.9345	3962.9346	-0.0001	2	1	2	2	1	1	0	1	1	1
4030.6108	4030.606	0.0048	6	2	4	6	6	6	1	5	6	6
4519.3026	4519.3017	0.0009	8	2	6	8	9	8	1	7	8	9
4574.9252	4574.9281	-0.0029	2	2	0	1	0	2	1	1	2	1
4576.6487	4576.6497	-0.001	2	2	0	3	3	2	1	1	3	3
4576.7811	4576.7809	0.0002	2	2	0	2	2	2	1	1	2	2
4576.7811	4576.7838	-0.0027	2	2	0	2	2	2	1	1	3	3
4576.5977	4576.5981	-0.0004	2	2	0	1	1	2	1	1	1	1
4576.497	4576.4914	0.0056	2	2	0	3	3	2	1	1	3	4
4576.4053	4576.4015	0.0038	2	2	0	3	3	2	1	1	3	2
4575.9867	4575.9867	0	2	2	0	2	3	2	1	1	2	2

4575.9867	4575.9897	-0.003	2	2	0	2	3	2	1	1	3	3
4575.3383	4575.3399	-0.0016	2	2	0	3	2	2	1	1	2	2
4575.1938	4575.1947	-0.0009	2	2	0	2	1	2	1	1	3	2
5003.0968	5003.0902	0.0066	3	1	3	3	2	2	0	2	2	1
5002.9884	5002.9901	-0.0017	3	1	3	3	2	2	0	2	3	2
5003.6508	5003.6549	-0.0041	3	1	3	2	3	2	0	2	2	3
5004.4301	5004.4316	-0.0015	3	1	3	3	2	2	0	2	2	2
5004.5218	5004.5265	-0.0047	3	1	3	4	3	2	0	2	3	3
5078.5919	5078.5987	-0.0068	9	2	7	9	10	9	1	8	9	10
5078.4826	5078.4878	-0.0052	9	2	7	10	11	9	1	8	10	11
5116.628	5116.6232	0.0048	2	2	1	3	2	2	1	2	3	2
5116.7185	5116.7184	0.0001	2	2	1	2	1	2	1	2	3	2
5116.7185	5116.7159	0.0026	2	2	1	3	2	2	1	2	2	1
5116.5575	5116.5609	-0.0034	2	2	1	1	0	2	1	2	2	1
5116.5575	5116.5617	-0.0042	2	2	1	2	1	2	1	2	1	0
5117.2167	5117.2164	0.0003	2	2	1	1	2	2	1	2	1	2
5117.3865	5117.3858	0.0007	2	2	1	3	4	2	1	2	3	4
5117.7845	5117.7867	-0.0022	2	2	1	2	3	2	1	2	2	3
5118.8167	5118.8195	-0.0028	2	2	1	1	1	2	1	2	1	1
5118.9168	5118.9185	-0.0017	2	2	1	3	3	2	1	2	3	3
5119.1743	5119.177	-0.0027	2	2	1	2	2	2	1	2	2	2
5118.2289	5118.2297	-0.0008	2	2	1	3	3	2	1	2	3	4
5323.1219	5323.12	0.0019	7	1	6	7	8	7	0	7	7	8
5323.0445	5323.0494	-0.0049	7	1	6	7	6	7	0	7	7	6
5323.5889	5323.5895	-0.0006	7	1	6	7	7	7	0	7	7	7
5323.3729	5323.3728	0.0001	7	1	6	8	8	7	0	7	8	8
5322.8325	5322.8322	0.0003	7	1	6	8	7	7	0	7	8	7
5796.1933	5796.1907	0.0026	4	2	3	4	4	4	1	4	4	4
5795.54	5795.5366	0.0034	4	2	3	4	5	4	1	4	4	5
5795.3085	5795.303	0.0055	4	2	3	5	6	4	1	4	5	6
5794.9437	5794.948	-0.0043	4	2	3	5	5	4	1	4	5	6
5979.3704	5979.3721	-0.0017	4	1	4	3	2	3	0	3	3	2
5979.4463	5979.4434	0.0029	4	1	4	3	4	3	0	3	3	4
5979.2934	5979.296	-0.0026	4	1	4	3	3	3	0	3	3	3
5978.0843	5978.0888	-0.0045	4	1	4	5	5	3	0	3	4	5
5978.0843	5978.0872	-0.0029	4	1	4	3	3	3	0	3	2	3
6286.5776	6286.572	0.0056	5	2	4	5	6	5	1	5	5	6
6286.4603	6286.4549	0.0054	5	2	4	5	4	5	1	5	5	4
6286.9152	6286.9161	-0.0009	5	2	4	6	6	5	1	5	6	6
6287.1162	6287.1118	0.0044	5	2	4	5	5	5	1	5	5	5
6286.363	6286.3649	-0.0019	5	2	4	6	7	5	1	5	6	7
6287.25	6287.2562	-0.0062	5	2	4	6	6	5	1	5	5	5

6287.4561	6287.4608	-0.0047	5	2	4	6	7	5	1	5	6	6
6287.7658	6287.762	0.0038	5	2	4	5	4	5	1	5	5	5
6509.9817	6509.9801	0.0016	8	1	7	9	9	8	0	8	9	9
6509.5215	6509.5186	0.0029	8	1	7	9	10	8	0	8	9	10
7074.9672	7074.9622	0.005	7	3	4	8	7	7	2	5	8	7
7074.9672	7074.9628	0.0044	7	3	4	7	6	7	2	5	7	6
7074.9672	7074.9621	0.0051	7	3	4	6	5	7	2	5	6	5
7372.577	7372.5771	-0.0001	2	2	1	3	2	1	1	0	2	2
7373.4495	7373.4501	-0.0006	2	2	1	1	2	1	1	0	1	2
7373.9769	7373.9723	0.0046	2	2	1	2	2	1	1	0	2	2
7374.2613	7374.262	-0.0007	2	2	1	2	1	1	1	0	2	1
7374.5269	7374.5265	0.0004	2	2	1	3	3	1	1	0	2	3
7374.6018	7374.6013	0.0005	2	2	1	1	1	1	1	0	0	1
7372.7292	7372.7349	-0.0057	2	2	1	2	1	1	1	0	1	1
7372.4904	7372.4846	0.0058	2	2	1	1	0	1	1	0	1	1
7569.5022	7569.5013	0.0009	7	2	6	7	7	7	1	7	7	7
7569.0729	7569.0717	0.0012	7	2	6	7	8	7	1	7	7	8
7569.0076	7569.0074	0.0002	7	2	6	7	6	7	1	7	7	6
7575.0064	7575.0094	-0.003	2	2	0	3	2	1	1	1	2	2
7574.8398	7574.8431	-0.0033	2	2	0	1	0	1	1	1	2	1
7576.4478	7576.4475	0.0003	2	2	0	2	2	1	1	1	2	1
7699.9445	7699.9441	0.0004	5	3	2	6	6	5	2	3	6	6
5078.7125	5078.7175	-0.005	9	2	7	8	8	9	1	8	8	8
6510.1912	6510.1941	-0.0029	8	1	7	8	8	8	0	8	8	8
6509.7375	6509.7372	0.0003	8	1	7	8	9	8	0	8	8	9
6509.4625	6509.4632	-0.0007	8	1	7	9	8	8	0	8	9	8
4174.7819	4174.7794	0.0025	4	2	2	5	6	4	1	3	5	6
2381.1375	2381.1407	-0.0032	7	2	5	7	8	6	3	4	6	7
4370.527	4370.5272	-0.0002	3	2	1	4	3	3	1	2	4	3
7576.3154	7576.3162	-0.0008	2	2	0	3	3	1	1	1	2	2
5003.215	5003.2193	-0.0043	3	1	3	4	3	2	0	2	3	2
7860.161	7860.1638	-0.0028	6	1	6	7	8	5	0	5	6	7
7860.161	7860.1637	-0.0027	6	1	6	5	6	5	0	5	4	5
7860.007	7860.0043	0.0027	6	1	6	6	6	5	0	5	5	5
4175.0375	4175.0329	0.0046	4	2	2	5	5	4	1	3	5	5
6107.6144	6107.614	0.0004	11	3	8	11	12	11	2	9	11	12
6107.7	6107.6983	0.0017	11	3	8	11	11	11	2	9	11	11
5979.0125	5979.0136	-0.0011	4	1	4	5	5	3	0	3	4	4
5978.9231	5978.9237	-0.0006	4	1	4	4	4	3	0	3	3	3
2344.775	2344.7756	-0.0006	9	2	8	10	11	8	3	5	9	10
3961.7345	3961.7331	0.0014	2	1	2	2	3	1	0	1	2	3
2730.4356	2730.4365	-0.0009	4	1	3	5	4	4	0	4	5	4

5322.9	5322.8971	0.0029	7	1	6	8	9	7	0	7	8	9
2240.2125	2240.2101	0.0024	3	1	2	4	4	3	0	3	4	4
2240.1625	2240.1603	0.0022	3	1	2	2	2	3	0	3	2	2
2239.6125	2239.6152	-0.0027	3	1	2	2	3	3	0	3	2	3
2239.5	2239.5038	-0.0038	3	1	2	4	3	3	0	3	4	3
2239.675	2239.6727	0.0023	3	1	2	4	5	3	0	3	4	5
6286.2575	6286.2595	-0.002	5	2	4	6	5	5	1	5	6	5
2528.5814	2528.5808	0.0006	3	0	3	2	3	2	1	2	1	2
5795.249	5795.2507	-0.0017	4	2	3	3	4	4	1	4	3	4
5795.1375	5795.1421	-0.0046	4	2	3	5	4	4	1	4	5	4
7576.5943	7576.5951	-0.0008	2	2	0	2	2	1	1	1	0	1
2157.7936	2157.7915	0.0021	12	4	8	12	11	11	5	7	11	10
2157.6089	2157.6054	0.0035	12	4	8	12	12	11	5	7	11	11
2239.2875	2239.2853	0.0022	3	1	2	4	4	3	0	3	4	5
2239.1469	2239.1447	0.0022	3	1	2	3	3	3	0	3	3	2
2238.9875	2238.986	0.0015	3	1	2	4	4	3	0	3	4	3
2840.7027	2840.7021	0.0006	10	2	9	10	10	9	3	6	9	9
3045.6353	3045.6323	0.003	11	2	10	11	12	10	3	7	10	11
3406.8386	3406.8396	-0.001	5	1	4	6	6	5	0	5	5	5
3407.1035	3407.1004	0.0031	5	1	4	6	7	5	0	5	6	6
3407.2125	3407.212	0.0005	5	1	4	6	5	5	0	5	6	6
3407.4125	3407.4109	0.0016	5	1	4	5	4	5	0	5	5	5
3405.4875	3405.4879	-0.0004	5	1	4	6	6	5	0	5	6	7
4767.7927	4767.7915	0.0012	6	1	5	5	4	5	2	4	4	3
5004.3	5004.2973	0.0027	3	1	3	3	2	2	0	2	3	3
5004.6	5004.6005	-0.0005	3	1	3	2	1	2	0	2	1	1
5402.75	5402.7529	-0.0029	5	0	5	5	6	4	1	4	4	5
5402.7	5402.7018	-0.0018	5	0	5	6	5	4	1	4	5	4
5402.425	5402.4242	0.0008	5	0	5	5	5	4	1	4	5	5
5403.075	5403.0773	-0.0023	5	0	5	4	3	4	1	4	4	3
5403.9724	5403.9736	-0.0012	5	0	5	5	4	4	1	4	4	4
5866.3933	5866.3967	-0.0034	10	2	8	9	10	10	1	9	9	10
5980.2043	5980.203	0.0013	4	1	4	4	3	3	0	3	3	3
5979.9262	5979.927	-0.0008	4	1	4	4	3	3	0	3	2	2
5980.2912	5980.2901	0.0011	4	1	4	5	4	3	0	3	4	4
5980.5	5980.5016	-0.0016	4	1	4	5	4	3	0	3	3	3
6266.4249	6266.424	0.0009	12	3	9	13	12	12	2	10	13	12
6266.5403	6266.5423	-0.002	12	3	9	11	11	12	2	10	11	11
6285.6113	6285.6089	0.0024	5	2	4	6	6	5	1	5	6	5
6286.0375	6286.0361	0.0014	5	2	4	5	5	5	1	5	5	6
6778.7531	6778.7539	-0.0008	6	0	6	5	5	5	1	5	4	4
6878.6372	6878.6359	0.0013	6	2	5	7	6	6	1	6	7	6

6879.372	6879.3772	-0.0052	6	2	5	6	6	6	1	6	6	6
7421.225	7421.2243	0.0007	6	3	3	6	5	6	2	4	6	5
7568.8	7568.802	-0.002	7	2	6	6	5	7	1	7	6	5
7570.3525	7570.3503	0.0022	7	2	6	7	6	7	1	7	7	7
7575.1083	7575.1094	-0.0011	2	2	0	2	1	1	1	1	2	2
7699.5981	7699.6018	-0.0037	5	3	2	4	5	5	2	3	4	5
7783.0788	7783.0836	-0.0048	9	1	8	9	8	9	0	9	9	8
7783.3387	7783.3409	-0.0022	9	1	8	8	8	9	0	9	8	8
7859.6959	7859.6987	-0.0028	6	1	6	6	6	5	0	5	6	6
7859.7761	7859.777	-0.0009	6	1	6	6	5	5	0	5	6	5
7861.3261	7861.331	-0.0049	6	1	6	6	5	5	0	5	5	5
7861.3922	7861.3943	-0.0021	6	1	6	7	6	5	0	5	6	6
7889.0415	7889.0436	-0.0021	4	3	1	3	2	4	2	2	3	2
7889.2081	7889.2084	-0.0003	4	3	1	4	3	4	2	2	4	3
7889.7678	7889.7668	0.001	4	3	1	3	3	4	2	2	3	3

Table S24: List of lines assigned for the C1 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2524.344	2524.3347	0.0093	3	0	3	3	2	2	1	2	2	1
2524.243	2524.2411	0.0019	3	0	3	4	4	2	1	2	3	3
2524.1739	2524.1628	0.0111	3	0	3	3	3	2	1	2	2	2
2729.476	2729.4733	0.0027	4	1	3	4	4	4	0	4	4	4
2729.2799	2729.2881	-0.0082	4	1	3	5	5	4	0	4	5	5
2729.0131	2729.0093	0.0038	4	1	3	4	5	4	0	4	4	5
2728.8749	2728.8768	-0.0019	4	1	3	4	3	4	0	4	4	3
2728.8001	2728.8068	-0.0067	4	1	3	5	6	4	0	4	5	6
2728.7037	2728.6938	0.0099	4	1	3	5	4	4	0	4	5	4
2833.1093	2833.1212	-0.0119	1	1	1	1	1	0	0	0	1	2
2833.3562	2833.3532	0.003	1	1	1	2	3	0	0	0	1	2
2833.5028	2833.5048	-0.002	1	1	1	2	2	0	0	0	1	2
3403.5701	3403.5603	0.0098	5	1	4	5	5	5	0	5	5	5
3403.3535	3403.3588	-0.0053	5	1	4	6	6	5	0	5	6	6
3403.101	3403.1003	0.0007	5	1	4	5	6	5	0	5	5	6
3403.0022	3402.9994	0.0028	5	1	4	5	4	5	0	5	5	4
3402.8828	3402.8873	-0.0045	5	1	4	6	7	5	0	5	6	7
3402.7981	3402.7983	-0.0002	5	1	4	6	5	5	0	5	6	5
3402.757	3402.7479	0.0091	5	1	4	4	3	5	0	5	4	3
3960.6845	3960.6862	-0.0017	2	1	2	3	3	1	0	1	2	2
3960.8782	3960.883	-0.0048	2	1	2	1	1	1	0	1	1	0

3960.7849	3960.7826	0.0023	2	1	2	1	2	1	0	1	1	2
3960.5422	3960.547	-0.0048	2	1	2	3	4	1	0	1	2	3
3959.8593	3959.8627	-0.0034	2	1	2	3	3	1	0	1	2	3
3959.7644	3959.7585	0.0059	2	1	2	3	2	1	0	1	2	1
3959.6688	3959.6659	0.0029	2	1	2	2	1	1	0	1	2	1
3972.1475	3972.1431	0.0044	4	0	4	5	6	3	1	3	4	5
4031.4562	4031.4524	0.0038	6	2	4	6	6	6	1	5	6	6
4031.4019	4031.4021	-0.0002	6	2	4	7	7	6	1	5	7	7
4031.2876	4031.281	0.0066	6	2	4	6	7	6	1	5	6	7
4045.3922	4045.4011	-0.0089	5	2	3	6	7	5	1	4	6	7
4045.5909	4045.5866	0.0043	5	2	3	6	5	5	1	4	5	6
4271.179	4271.1799	-0.0009	6	1	5	6	6	6	0	6	6	6
4270.9642	4270.9662	-0.002	6	1	5	7	7	6	0	6	7	7
4270.7108	4270.717	-0.0062	6	1	5	6	7	6	0	6	6	7
4270.6433	4270.6344	0.0089	6	1	5	6	5	6	0	6	6	5
4270.488	4270.4951	-0.0071	6	1	5	7	8	6	0	6	7	8
4270.4251	4270.4205	0.0046	6	1	5	7	6	6	0	6	7	6
4372.507	4372.5168	-0.0098	3	2	1	4	3	3	1	2	4	3
4372.6643	4372.6687	-0.0044	3	2	1	4	5	3	1	2	4	5
4372.7514	4372.7495	0.0019	3	2	1	3	4	3	1	2	3	4
4373.189	4373.1933	-0.0043	3	2	1	3	3	3	1	2	3	3
4373.1278	4373.1258	0.002	3	2	1	4	4	3	1	2	4	4
4577.6177	4577.6112	0.0065	2	2	0	2	3	2	1	1	2	3
4578.4402	4578.4444	-0.0042	2	2	0	3	3	2	1	1	3	3
4578.5757	4578.5731	0.0026	2	2	0	2	2	2	1	1	2	2
4577.4054	4577.4107	-0.0053	2	2	0	3	4	2	1	1	3	4
4577.3275	4577.3266	0.0009	2	2	0	1	2	2	1	1	1	2
4757.1075	4757.1148	-0.0073	6	1	5	7	8	5	2	4	6	7
4757.0357	4757.0317	0.004	6	1	5	7	7	5	2	4	6	6
5001.2685	5001.2606	0.0079	3	1	3	4	5	2	0	2	3	4
5001.1899	5001.1846	0.0053	3	1	3	3	4	2	0	2	2	3
5001.1237	5001.1163	0.0074	3	1	3	4	3	2	0	2	3	2
5976.3639	5976.3596	0.0043	4	1	4	5	6	3	0	3	4	5
5976.1764	5976.1684	0.008	4	1	4	4	4	3	0	3	3	3
6771.8482	6771.8562	-0.008	6	0	6	7	8	5	1	5	6	7
6916.5192	6916.5082	0.011	5	1	5	5	5	4	0	4	4	4
6916.5955	6916.5862	0.0093	5	1	5	6	6	4	0	4	5	5
7574.4396	7574.4454	-0.0058	2	2	0	3	4	1	1	1	2	3
7574.6502	7574.6599	-0.0097	2	2	0	2	3	1	1	1	1	2
7574.3561	7574.3556	0.0005	2	2	0	1	2	1	1	1	0	1
7574.2247	7574.2404	-0.0157	2	2	0	3	2	1	1	1	1	1
7855.8809	7855.8774	0.0035	6	1	6	7	8	5	0	5	6	7

7855.775	7855.7827	-0.0077	6	1	6	7	7	5	0	5	6	6
2524.4875	2524.4807	0.0068	3	0	3	4	5	2	1	2	3	4
4176.7808	4176.7753	0.0055	4	2	2	5	6	4	1	3	5	6
4177.0311	4177.0407	-0.0096	6	0	6	5	4	3	3	1	4	4

Table S25: List of lines assigned for the C2 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2223.5915	2223.5899	0.0016	3	1	2	3	3	3	0	3	3	3
2222.7147	2222.722	-0.0073	3	1	2	4	3	3	0	3	4	3
2222.6208	2222.6334	-0.0126	3	1	2	2	1	3	0	3	2	1
2542.0026	2541.9979	0.0047	3	0	3	3	3	2	1	2	2	2
2542.0738	2542.0764	-0.0026	3	0	3	4	4	2	1	2	3	3
2541.8735	2541.8667	0.0068	3	0	3	3	3	2	1	2	3	3
2542.3238	2542.3164	0.0074	3	0	3	4	5	2	1	2	3	4
2719.4441	2719.4351	0.009	4	1	3	4	4	4	0	4	4	4
2719.2502	2719.2494	0.0008	4	1	3	5	5	4	0	4	5	5
2718.9726	2718.9686	0.004	4	1	3	4	5	4	0	4	4	5
2718.8456	2718.8354	0.0102	4	1	3	4	3	4	0	4	4	3
2718.7726	2718.7656	0.007	4	1	3	5	6	4	0	4	5	6
2718.6607	2718.6519	0.0088	4	1	3	5	4	4	0	4	5	4
2718.5942	2718.589	0.0052	4	1	3	3	2	4	0	4	3	2
2808.6293	2808.6223	0.007	1	1	1	1	1	0	0	0	1	2
2808.8539	2808.853	0.0009	1	1	1	2	3	0	0	0	1	2
2809.0065	2809.0037	0.0028	1	1	1	2	2	0	0	0	1	2
3071.1141	3071.1102	0.0039	5	1	4	6	6	4	2	3	5	5
3071.3315	3071.3264	0.0051	5	1	4	6	7	4	2	3	5	6
3401.9332	3401.9268	0.0064	5	1	4	5	5	5	0	5	5	5
3401.7336	3401.7248	0.0088	5	1	4	6	6	5	0	5	6	6
3401.4715	3401.4642	0.0073	5	1	4	5	6	5	0	5	5	6
3401.363	3401.3627	0.0003	5	1	4	5	4	5	0	5	5	4
3401.2449	3401.2506	-0.0057	5	1	4	6	7	5	0	5	6	7
3401.1721	3401.1611	0.011	5	1	4	6	5	5	0	5	6	5
3932.3854	3932.3833	0.0021	2	1	2	3	2	1	0	1	2	1
3932.4848	3932.4862	-0.0014	2	1	2	3	3	1	0	1	2	3
3932.292	3932.2909	0.0011	2	1	2	2	1	1	0	1	2	1
3933.1686	3933.1712	-0.0026	2	1	2	3	4	1	0	1	2	3
3933.317	3933.3092	0.0078	2	1	2	3	3	1	0	1	2	2
3933.4103	3933.406	0.0043	2	1	2	1	2	1	0	1	1	2
3933.5148	3933.5055	0.0093	2	1	2	1	1	1	0	1	1	0

3984.1555	3984.1524	0.0031	5	2	3	6	7	5	1	4	6	7
3984.3563	3984.3419	0.0144	5	2	3	6	6	5	1	4	6	6
3986.5954	3986.6078	-0.0124	4	0	4	4	4	3	1	3	3	3
3986.6933	3986.6981	-0.0048	4	0	4	5	6	3	1	3	4	5
4110.2501	4110.258	-0.0079	4	2	2	4	5	4	1	3	4	5
4110.2217	4110.213	0.0087	4	2	2	5	6	4	1	3	5	6
4110.1554	4110.1493	0.0061	4	2	2	5	4	4	1	3	5	4
4278.6001	4278.598	0.0021	6	1	5	7	8	6	0	6	7	8
4278.7356	4278.7372	-0.0016	6	1	5	6	5	6	0	6	6	5
4278.8143	4278.8202	-0.0059	6	1	5	6	7	6	0	6	6	7
4279.0671	4279.0714	-0.0043	6	1	5	7	7	6	0	6	7	7
4279.2877	4279.2854	0.0023	6	1	5	6	6	6	0	6	6	6
4304.0741	4304.0732	0.0009	3	2	1	3	4	3	1	2	3	4
4303.9972	4303.9922	0.005	3	2	1	4	5	3	1	2	4	5
4303.8326	4303.8402	-0.0076	3	2	1	4	3	3	1	2	4	3
4304.5251	4304.5175	0.0076	3	2	1	3	3	3	1	2	3	3
4304.4611	4304.4498	0.0113	3	2	1	4	4	3	1	2	4	4
4494.3804	4494.3933	-0.0129	8	2	6	9	10	8	1	7	9	10
4494.4856	4494.4866	-0.001	8	2	6	8	9	8	1	7	8	9
4494.6	4494.6065	-0.0065	8	2	6	9	9	8	1	7	9	9
4494.6823	4494.6977	-0.0154	8	2	6	8	8	8	1	7	8	8
4508.1899	4508.1919	-0.002	2	2	0	3	2	2	1	1	3	2
4508.6299	4508.6382	-0.0083	2	2	0	1	2	2	1	1	1	2
4508.7178	4508.722	-0.0042	2	2	0	3	4	2	1	1	3	4
4508.923	4508.9219	0.0011	2	2	0	2	3	2	1	1	2	3
4509.7628	4509.755	0.0078	2	2	0	3	3	2	1	1	3	3
4509.8914	4509.8833	0.0081	2	2	0	2	2	2	1	1	2	2
4509.6885	4509.7047	-0.0162	2	2	0	1	1	2	1	1	1	1
4822.8359	4822.8506	-0.0147	6	1	5	7	8	5	2	4	6	7
4822.7551	4822.7671	-0.012	6	1	5	7	7	5	2	4	6	6
4970.4839	4970.4915	-0.0076	3	1	3	4	5	2	0	2	3	4
4970.4151	4970.4156	-0.0005	3	1	3	3	4	2	0	2	2	3
4970.3406	4970.3473	-0.0067	3	1	3	4	3	2	0	2	3	2
4970.2258	4970.2181	0.0077	3	1	3	3	2	2	0	2	2	1
5736.1202	5736.1255	-0.0053	4	2	3	4	5	4	1	4	4	5
5736.572	5736.5622	0.0098	4	2	3	5	5	4	1	4	5	5
5735.897	5735.8921	0.0049	4	2	3	5	6	4	1	4	5	6
5735.7372	5735.7322	0.005	4	2	3	5	4	4	1	4	5	4
5735.6668	5735.6598	0.007	4	2	3	3	2	4	1	4	3	2
5942.1223	5942.1068	0.0155	4	1	4	4	4	3	0	3	3	3
5942.3015	5942.2976	0.0039	4	1	4	5	6	3	0	3	4	5
6230.2631	6230.2637	-0.0006	5	2	4	6	7	5	1	5	6	7

6230.3508	6230.355	-0.0042	5	2	4	5	4	5	1	5	5	4
6230.474	6230.4712	0.0028	5	2	4	5	6	5	1	5	5	6
6230.1511	6230.1593	-0.0082	5	2	4	6	5	5	1	5	6	5
6230.8196	6230.8105	0.0091	5	2	4	6	6	5	1	5	6	6
6231.0085	6231.0066	0.0019	5	2	4	5	5	5	1	5	5	5
6774.5131	6774.5061	0.007	6	0	6	7	7	5	1	5	6	6
7302.4455	7302.4452	0.0003	2	2	1	3	3	1	1	0	2	2
7302.5727	7302.5704	0.0023	2	2	1	2	2	1	1	0	2	2
7302.6371	7302.6328	0.0043	2	2	1	2	2	1	1	0	1	1
7302.763	7302.757	0.006	2	2	1	3	2	1	1	0	2	1
7302.8496	7302.8512	-0.0016	2	2	1	2	1	1	1	0	2	1
7505.9408	7505.9369	0.0039	2	2	0	2	3	1	1	1	1	2
7505.7279	7505.7226	0.0053	2	2	0	3	4	1	1	1	2	3
7505.5177	7505.5161	0.0016	2	2	0	3	2	1	1	1	1	1
7506.4447	7506.4423	0.0024	2	2	0	3	3	1	1	1	2	2
7506.5606	7506.5705	-0.0099	2	2	0	2	2	1	1	1	2	1
7775.7668	7775.7839	-0.0171	4	3	1	4	5	4	2	2	4	5
7776.325	7776.3436	-0.0186	4	3	1	4	4	4	2	2	4	4
7818.2757	7818.2799	-0.0042	6	1	6	7	7	5	0	5	6	6
7818.2757	7818.2806	-0.0049	6	1	6	5	5	5	0	5	4	4
7818.3714	7818.3736	-0.0022	6	1	6	7	8	5	0	5	6	7
7885.3206	7885.3382	-0.0176	3	3	0	4	4	3	2	1	4	4
7302.2904	7302.2788	0.0116	2	2	1	3	4	1	1	0	2	3
2223.0794	2223.0877	-0.0083	3	1	2	3	4	3	0	3	3	4
4110.4702	4110.4707	-0.0005	4	2	2	5	5	4	1	3	5	5

Table S26: List of lines assigned for the C3 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2207.7849	2207.7845	0.0004	3	1	2	3	3	3	0	3	3	3
2207.6224	2207.6156	0.0068	3	1	2	4	4	3	0	3	4	4
2207.2768	2207.2775	-0.0007	3	1	2	3	4	3	0	3	3	4
2207.0264	2207.019	0.0074	3	1	2	2	3	3	0	3	2	3
2206.9138	2206.9081	0.0057	3	1	2	4	3	3	0	3	4	3
2206.8287	2206.8186	0.0101	3	1	2	2	1	3	0	3	2	1
2563.6451	2563.6525	-0.0074	3	0	3	4	5	2	1	2	3	4
2563.5132	2563.5112	0.002	3	0	3	3	2	2	1	2	2	1
2563.4096	2563.4192	-0.0096	3	0	3	4	4	2	1	2	3	3
2563.3448	2563.3474	-0.0026	3	0	3	3	3	2	1	2	2	2
2710.7958	2710.7912	0.0046	4	1	3	4	4	4	0	4	4	4

2710.599	2710.6022	-0.0032	4	1	3	5	5	4	0	4	5	5
2710.3183	2710.3173	0.001	4	1	3	4	5	4	0	4	4	5
2710.1865	2710.1821	0.0044	4	1	3	4	3	4	0	4	4	3
2710.1042	2710.1105	-0.0063	4	1	3	5	6	4	0	4	5	6
2710.002	2709.9951	0.0069	4	1	3	5	4	4	0	4	5	4
2709.9391	2709.931	0.0081	4	1	3	3	2	4	0	4	3	2
2784.157	2784.1502	0.0068	1	1	1	2	2	0	0	0	1	2
2784.0133	2784.0096	0.0037	1	1	1	2	3	0	0	0	1	2
2783.7973	2783.7892	0.0081	1	1	1	1	1	0	0	0	1	2
3402.6442	3402.6439	0.0003	5	1	4	5	4	5	0	5	5	4
3403.002	3403.0121	-0.0101	5	1	4	6	6	5	0	5	6	6
3905.1807	3905.181	-0.0003	2	1	2	3	2	1	0	1	2	1
3905.2637	3905.2713	-0.0076	2	1	2	3	3	1	0	1	2	3
3905.0927	3905.0894	0.0033	2	1	2	2	1	1	0	1	2	1
3906.0932	3906.0834	0.0098	2	1	2	3	3	1	0	1	2	2
3905.948	3905.957	-0.009	2	1	2	3	4	1	0	1	2	3
3907.1178	3907.1062	0.0116	2	1	2	3	2	1	0	1	2	2
3920.3681	3920.3577	0.0104	5	2	3	6	7	5	1	4	6	7
3920.5603	3920.5471	0.0132	5	2	3	6	6	5	1	4	6	6
3925.5858	3925.5908	-0.005	6	2	4	7	8	6	1	5	7	8
3925.6575	3925.6452	0.0123	6	2	4	6	7	6	1	5	6	7
3925.7745	3925.7703	0.0042	6	2	4	7	7	6	1	5	7	7
3925.8318	3925.8224	0.0094	6	2	4	6	6	6	1	5	6	6
4005.3496	4005.3594	-0.0098	4	0	4	5	6	3	1	3	4	5
4005.3067	4005.2939	0.0128	4	0	4	5	5	3	1	3	4	4
4040.3893	4040.3977	-0.0084	4	2	2	5	6	4	1	3	5	6
4099.6424	4099.6315	0.0109	7	2	5	8	8	7	1	6	8	8
4231.8441	4231.8384	0.0057	3	2	1	4	5	3	1	2	4	5
4231.6825	4231.6884	-0.0059	3	2	1	4	3	3	1	2	4	3
4292.0274	4292.0348	-0.0074	6	1	5	6	6	6	0	6	6	6
4291.4714	4291.4759	-0.0045	6	1	5	6	5	6	0	6	6	5
4291.323	4291.3331	-0.0101	6	1	5	7	8	6	0	6	7	8
4940.264	4940.27	-0.006	3	1	3	4	5	2	0	2	3	4
4940.0056	4939.9994	0.0062	3	1	3	3	2	2	0	2	2	1
4986.4015	4986.3893	0.0122	2	2	1	2	3	2	1	2	2	3
4987.5318	4987.5239	0.0079	2	2	1	3	3	2	1	2	3	3
4987.4286	4987.428	0.0006	2	2	1	1	1	2	1	2	1	1
4985.2463	4985.2447	0.0016	2	2	1	3	2	2	1	2	3	2
4986.6891	4986.6895	-0.0004	2	2	1	3	4	2	1	2	3	3
4986.8365	4986.8382	-0.0017	2	2	1	3	3	2	1	2	3	4
5279.2901	5279.2919	-0.0018	3	2	2	4	3	3	1	3	4	3
5279.1764	5279.1674	0.009	3	2	2	2	1	3	1	3	2	1

5279.5914	5279.5852	0.0062	3	2	2	4	5	3	1	3	4	5
5280.7439	5280.736	0.0079	3	2	2	3	3	3	1	3	3	3
5419.8336	5419.8224	0.0112	5	0	5	6	7	4	1	4	5	6
5675.6228	5675.624	-0.0012	4	2	3	4	5	4	1	4	4	5
5676.0591	5676.0647	-0.0056	4	2	3	5	5	4	1	4	5	5
5676.287	5676.2762	0.0108	4	2	3	4	4	4	1	4	4	4
5675.3959	5675.3924	0.0035	4	2	3	5	6	4	1	4	5	6
5909.0455	5909.0497	-0.0042	4	1	4	5	5	3	0	3	4	4
6175.3507	6175.344	0.0067	5	2	4	6	6	5	1	5	6	6
6175.5412	6175.54	0.0012	5	2	4	5	5	5	1	5	5	5
6175.0124	6175.001	0.0114	5	2	4	5	6	5	1	5	5	6
6174.7883	6174.7937	-0.0054	5	2	4	6	7	5	1	5	6	7
6174.6785	6174.6885	-0.01	5	2	4	6	5	5	1	5	6	5
6781.7952	6781.8068	-0.0116	6	0	6	7	8	5	1	5	6	7
6844.9627	6844.9621	0.0006	5	1	5	5	5	4	0	4	4	4
6845.1602	6845.151	0.0092	5	1	5	6	7	4	0	4	5	6
7230.2759	7230.2717	0.0042	2	2	1	3	3	1	1	0	2	2
7230.5951	7230.5976	-0.0025	2	2	1	3	2	1	1	0	2	1
7230.6862	7230.6874	-0.0012	2	2	1	2	1	1	1	0	2	1
7230.9515	7230.9493	0.0022	2	2	1	3	3	1	1	0	2	3
7435.626	7435.6315	-0.0055	2	2	0	3	2	1	1	1	1	1
7435.7561	7435.7577	-0.0016	2	2	0	1	2	1	1	1	0	1
7435.8506	7435.8457	0.0049	2	2	0	3	4	1	1	1	2	3
7436.0613	7436.0574	0.0039	2	2	0	2	3	1	1	1	1	2
7436.5568	7436.5671	-0.0103	2	2	0	3	3	1	1	1	2	2
7653.9126	7653.9262	-0.0136	4	3	1	5	5	4	2	2	5	5
7654.0314	7654.0355	-0.0041	4	3	1	4	4	4	2	2	4	4
7765.5165	7765.5159	0.0006	3	3	0	3	4	3	2	1	3	4
7766.4693	7766.4824	-0.0131	3	3	0	3	3	3	2	1	3	3
7848.7227	7848.7314	-0.0087	3	3	1	3	4	3	2	2	3	4
7849.7463	7849.761	-0.0147	3	3	1	3	3	3	2	2	3	3
7847.9949	7848.0003	-0.0054	3	3	1	2	1	3	2	2	2	1
7847.9949	7848.0002	-0.0053	3	3	1	2	1	3	2	2	3	2
7892.9899	7892.9971	-0.0072	4	3	2	5	4	4	2	3	5	4
7893.7992	7893.7963	0.0029	4	3	2	3	3	4	2	3	3	3
7230.1149	7230.1149	0	2	2	1	3	4	1	1	0	2	3
5280.4996	5280.5009	-0.0013	3	2	2	4	4	3	1	3	4	4
3402.4961	3402.489	0.0071	5	1	4	4	5	5	0	5	4	5
4040.445	4040.4375	0.0075	4	2	2	4	5	4	1	3	4	5
4040.6553	4040.6517	0.0036	4	2	2	5	5	4	1	3	5	5

Table S27: List of lines assigned for the C4 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2223.0706	2223.0592	0.0114	3	1	2	3	4	3	0	3	3	4
2222.8099	2222.8023	0.0076	3	1	2	2	3	3	0	3	2	3
2223.3974	2223.3989	-0.0015	3	1	2	4	4	3	0	3	4	4
2223.3401	2223.3488	-0.0087	3	1	2	2	2	3	0	3	2	2
2715.6878	2715.6812	0.0066	4	1	3	4	4	4	0	4	4	4
2715.4962	2715.4955	0.0007	4	1	3	5	5	4	0	4	5	5
2715.2088	2715.2068	0.002	4	1	3	4	5	4	0	4	4	5
2715.081	2715.0715	0.0095	4	1	3	4	3	4	0	4	4	3
2714.997	2715.0038	-0.0068	4	1	3	5	6	4	0	4	5	6
2714.8281	2714.8252	0.0029	4	1	3	3	2	4	0	4	3	2
2810.6023	2810.6041	-0.0018	1	1	1	2	2	0	0	0	1	2
2810.464	2810.465	-0.001	1	1	1	2	3	0	0	0	1	2
2810.2581	2810.2526	0.0055	1	1	1	1	1	0	0	0	1	2
3393.0019	3392.9967	0.0052	5	1	4	5	5	5	0	5	5	5
3392.8002	3392.7948	0.0054	5	1	4	6	6	5	0	5	6	6
3392.5263	3392.5245	0.0018	5	1	4	5	6	5	0	5	5	6
3392.428	3392.421	0.007	5	1	4	5	4	5	0	5	5	4
3392.3074	3392.311	-0.0036	5	1	4	6	7	5	0	5	6	7
3932.8803	3932.8766	0.0037	2	1	2	3	3	1	0	1	2	2
3933.9073	3933.8992	0.0081	2	1	2	3	2	1	0	1	2	2
3932.7369	3932.7495	-0.0126	2	1	2	3	4	1	0	1	2	3
3931.9841	3931.9782	0.0059	2	1	2	3	2	1	0	1	2	1
3932.0508	3932.0634	-0.0126	2	1	2	3	3	1	0	1	2	3
3931.8889	3931.8853	0.0036	2	1	2	2	1	1	0	1	2	1
3969.9236	3969.9266	-0.003	4	0	4	5	6	3	1	3	4	5
3988.1755	3988.1728	0.0027	6	2	4	7	7	6	1	5	7	7
3988.0624	3988.0528	0.0096	6	2	4	6	7	6	1	5	6	7
3987.9948	3987.9988	-0.004	6	2	4	7	8	6	1	5	7	8
3988.2255	3988.2246	0.0009	6	2	4	6	6	6	1	5	6	6
3996.6333	3996.6316	0.0017	5	2	3	6	7	5	1	4	6	7
4124.6803	4124.6707	0.0096	4	2	2	5	5	4	1	3	5	5
4124.4279	4124.4223	0.0056	4	2	2	5	6	4	1	3	5	6
4264.1272	4264.1264	0.0008	6	1	5	6	6	6	0	6	6	6
4263.9117	4263.9127	-0.001	6	1	5	7	7	6	0	6	7	7
4263.6386	4263.6504	-0.0118	6	1	5	6	7	6	0	6	6	7
4263.5738	4263.5655	0.0083	6	1	5	6	5	6	0	6	6	5
4263.4262	4263.4283	-0.0021	6	1	5	7	8	6	0	6	7	8
4318.578	4318.5772	0.0008	3	2	1	3	4	3	1	2	3	4

4318.4919	4318.4938	-0.0019	3	2	1	4	5	3	1	2	4	5
4318.3345	4318.347	-0.0125	3	2	1	4	3	3	1	2	4	3
4319.0077	4319.0067	0.001	3	2	1	3	3	3	1	2	3	3
4318.9365	4318.937	-0.0005	3	2	1	4	4	3	1	2	4	4
4968.4796	4968.4797	-0.0001	3	1	3	4	5	2	0	2	3	4
4968.4103	4968.4042	0.0061	3	1	3	3	4	2	0	2	2	3
4968.2191	4968.2111	0.008	3	1	3	3	2	2	0	2	2	1
5064.3578	5064.3593	-0.0015	2	2	1	3	4	2	1	2	3	4
5064.1848	5064.189	-0.0042	2	2	1	1	2	2	1	2	1	2
5064.7485	5064.7613	-0.0128	2	2	1	2	3	2	1	2	2	3
5065.8681	5065.8781	-0.01	2	2	1	3	3	2	1	2	3	3
5065.7772	5065.7792	-0.002	2	2	1	1	1	2	1	2	1	1
5066.1321	5066.1376	-0.0055	2	2	1	2	2	2	1	2	2	2
5063.6044	5063.6047	-0.0003	2	2	1	3	2	2	1	2	3	2
5352.9742	5352.9705	0.0037	3	2	2	4	3	3	1	3	4	3
5352.8422	5352.8426	-0.0004	3	2	2	2	1	3	1	3	2	1
5353.2654	5353.2628	0.0026	3	2	2	4	5	3	1	3	4	5
5353.5473	5353.5488	-0.0015	3	2	2	3	4	3	1	3	3	4
5354.1803	5354.1775	0.0028	3	2	2	4	4	3	1	3	4	4
5354.1064	5354.1056	0.0008	3	2	2	2	2	3	1	3	2	2
5354.4199	5354.4193	0.0006	3	2	2	3	3	3	1	3	3	3
5742.6896	5742.6868	0.0028	4	2	3	5	6	4	1	4	5	6
5742.5265	5742.5265	0	4	2	3	5	4	4	1	4	5	4
5742.9083	5742.9217	-0.0134	4	2	3	4	5	4	1	4	4	5
5938.8331	5938.8374	-0.0043	4	1	4	5	6	3	0	3	4	5
5938.6494	5938.6392	0.0102	4	1	4	4	4	3	0	3	3	3
6234.0451	6234.0556	-0.0105	5	2	4	6	7	5	1	5	6	7
6234.8037	6234.8033	0.0004	5	2	4	5	5	5	1	5	5	5
6234.605	6234.6063	-0.0013	5	2	4	6	6	5	1	5	6	6
6233.9531	6233.9504	0.0027	5	2	4	6	5	5	1	5	6	5
6233.9013	6233.901	0.0003	5	2	4	4	3	5	1	5	4	3
6616.4619	6616.4528	0.0091	8	3	5	9	10	8	2	6	9	10
6754.5626	6754.5665	-0.0039	6	0	6	7	7	5	1	5	6	6
6874.8734	6874.871	0.0024	5	1	5	5	5	4	0	4	4	4
7309.3015	7309.2994	0.0021	2	2	1	3	3	1	1	0	2	2
7309.4966	7309.4893	0.0073	2	2	1	2	2	1	1	0	1	1
7309.636	7309.632	0.004	2	2	1	3	2	1	1	0	2	1
7511.278	7511.2775	0.0005	2	2	0	3	4	1	1	1	2	3
7511.4889	7511.4931	-0.0042	2	2	0	2	3	1	1	1	1	2
7511.186	7511.1871	-0.0011	2	2	0	1	2	1	1	1	0	1
7511.0526	7511.0592	-0.0066	2	2	0	3	2	1	1	1	1	1
7511.9912	7511.9982	-0.007	2	2	0	3	3	1	1	1	2	2

7512.1346	7512.1294	0.0052	2	2	0	2	2	1	1	1	2	1
7810.9611	7810.9762	-0.0151	6	1	6	7	8	5	0	5	6	7
5938.7334	5938.7297	0.0037	4	1	4	5	5	3	0	3	4	4
5387.2175	5387.2206	-0.0031	5	0	5	6	6	4	1	4	5	5
6874.9592	6874.9484	0.0108	5	1	5	6	6	4	0	4	5	5
4263.3559	4263.3515	0.0044	6	1	5	7	6	6	0	6	7	6

Table S28: List of lines assigned for the C5 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2238.1231	2238.1188	0.0043	3	1	2	3	3	3	0	3	3	3
2237.9559	2237.9523	0.0036	3	1	2	4	4	3	0	3	4	4
2237.6199	2237.614	0.0059	3	1	2	3	4	3	0	3	3	4
2237.4165	2237.417	-0.0005	3	1	2	4	5	3	0	3	4	5
2237.2556	2237.2488	0.0068	3	1	2	4	3	3	0	3	4	3
2513.6914	2513.6922	-0.0008	3	0	3	2	1	2	1	2	2	1
2513.3843	2513.3796	0.0047	3	0	3	3	2	2	1	2	2	1
2513.2172	2513.2155	0.0017	3	0	3	3	3	2	1	2	2	2
2725.1954	2725.1933	0.0021	4	1	3	4	4	4	0	4	4	4
2725.0044	2725.0094	-0.005	4	1	3	5	5	4	0	4	5	5
2724.7261	2724.7236	0.0025	4	1	3	4	5	4	0	4	4	5
2724.5983	2724.5897	0.0086	4	1	3	4	3	4	0	4	4	3
2724.5119	2724.5224	-0.0105	4	1	3	5	6	4	0	4	5	6
2724.3465	2724.3456	0.0009	4	1	3	3	2	4	0	4	3	2
2832.4392	2832.4382	0.001	1	1	1	2	3	0	0	0	1	2
2832.2206	2832.216	0.0046	1	1	1	1	1	0	0	0	1	2
2832.5842	2832.5834	0.0008	1	1	1	2	2	0	0	0	1	2
3395.4661	3395.4631	0.003	5	1	4	5	5	5	0	5	5	5
3395.2613	3395.263	-0.0017	5	1	4	6	6	5	0	5	6	6
3395.0014	3394.9964	0.005	5	1	4	5	6	5	0	5	5	6
3394.8964	3394.8942	0.0022	5	1	4	5	4	5	0	5	5	4
3394.783	3394.7849	-0.0019	5	1	4	6	7	5	0	5	6	7
3394.6982	3394.6946	0.0036	5	1	4	6	5	5	0	5	6	5
3957.6452	3957.6413	0.0039	2	1	2	3	3	1	0	1	2	2
3957.5005	3957.5086	-0.0081	2	1	2	3	4	1	0	1	2	3
3956.7395	3956.7278	0.0117	2	1	2	3	2	1	0	1	2	1
3956.6353	3956.6355	-0.0002	2	1	2	2	1	1	0	1	2	1
3958.3495	3958.3475	0.002	4	0	4	5	6	3	1	3	4	5
3958.2971	3958.2842	0.0129	4	0	4	5	5	3	1	3	4	4
4034.5312	4034.523	0.0082	6	2	4	6	7	6	1	5	6	7

4034.4681	4034.4712	-0.0031	6	2	4	7	8	6	1	5	7	8
4034.6914	4034.693	-0.0016	6	2	4	6	6	6	1	5	6	6
4034.6546	4034.6434	0.0112	6	2	4	7	7	6	1	5	7	7
4051.0647	4051.0533	0.0114	5	2	3	6	6	5	1	4	6	6
4050.8743	4050.8693	0.005	5	2	3	6	7	5	1	4	6	7
4183.1675	4183.167	0.0005	4	2	2	5	4	4	1	3	5	4
4258.4198	4258.4254	-0.0056	6	1	5	6	6	6	0	6	6	6
4258.2069	4258.2133	-0.0064	6	1	5	7	7	6	0	6	7	7
4257.947	4257.9551	-0.0081	6	1	5	6	7	6	0	6	6	7
4257.86	4257.8713	-0.0113	6	1	5	6	5	6	0	6	6	5
4257.7371	4257.7347	0.0024	6	1	5	7	8	6	0	6	7	8
4257.6638	4257.6589	0.0049	6	1	5	7	6	6	0	6	7	6
4257.6275	4257.6168	0.0107	6	1	5	5	4	6	0	6	5	4
4379.2175	4379.2266	-0.0091	3	2	1	3	4	3	1	2	3	4
4379.1388	4379.1457	-0.0069	3	2	1	4	5	3	1	2	4	5
4379.601	4379.5955	0.0055	3	2	1	4	4	3	1	2	4	4
4379.6569	4379.6631	-0.0062	3	2	1	3	3	3	1	2	3	3
4584.3844	4584.3889	-0.0045	2	2	0	3	3	2	1	1	3	3
4583.5651	4583.5669	-0.0018	2	2	0	2	3	2	1	1	2	3
4583.3552	4583.3665	-0.0113	2	2	0	3	4	2	1	1	3	4
4728.2759	4728.2821	-0.0062	6	1	5	7	8	5	2	4	6	7
4728.2019	4728.2047	-0.0028	6	1	5	7	7	5	2	4	6	6
4728.2019	4728.1978	0.0041	6	1	5	5	5	5	2	4	4	4
4996.449	4996.4483	0.0007	3	1	3	4	5	2	0	2	3	4
4996.3023	4996.3068	-0.0045	3	1	3	4	3	2	0	2	3	2
4996.3688	4996.3729	-0.0041	3	1	3	3	4	2	0	2	2	3
5121.1717	5121.1635	0.0082	2	2	1	3	2	2	1	2	3	2
5121.7478	5121.755	-0.0072	2	2	1	1	2	2	1	2	1	2
5121.9191	5121.923	-0.0039	2	2	1	3	4	2	1	2	3	4
5122.3146	5122.3204	-0.0058	2	2	1	2	3	2	1	2	2	3
5122.1884	5122.1866	0.0018	2	2	1	3	2	2	1	2	3	3
5122.7656	5122.7624	0.0032	2	2	1	3	3	2	1	2	3	4
5123.3533	5123.3504	0.0029	2	2	1	1	1	2	1	2	1	1
5123.4523	5123.4486	0.0037	2	2	1	3	3	2	1	2	3	3
5123.7097	5123.7049	0.0048	2	2	1	2	2	2	1	2	2	2
5380.4303	5380.4204	0.0099	5	0	5	6	5	4	1	4	5	4
5408.4042	5408.4032	0.001	3	2	2	2	1	3	1	3	2	1
5408.5302	5408.5298	0.0004	3	2	2	4	3	3	1	3	4	3
5408.7383	5408.7404	-0.0021	3	2	2	2	3	3	1	3	2	3
5408.8245	5408.8231	0.0014	3	2	2	4	5	3	1	3	4	5
5409.1037	5409.1062	-0.0025	3	2	2	3	4	3	1	3	3	4
5409.6685	5409.6684	0.0001	3	2	2	2	2	3	1	3	2	2

5409.7435	5409.7397	0.0038	3	2	2	4	4	3	1	3	4	4
5409.9813	5409.9788	0.0025	3	2	2	3	3	3	1	3	3	3
5969.9193	5969.9167	0.0026	4	1	4	5	6	3	0	3	4	5
6727.2459	6727.2449	0.001	8	3	5	9	10	8	2	6	9	10
6727.311	6727.3094	0.0016	8	3	5	9	9	8	2	6	9	9
6753.9533	6753.9639	-0.0106	6	0	6	7	8	5	1	5	6	7
7573.544	7573.5537	-0.0097	2	2	0	3	3	1	1	1	2	2
7573.6871	7573.6823	0.0048	2	2	0	2	2	1	1	1	2	1
7573.0427	7573.0467	-0.004	2	2	0	2	3	1	1	1	1	2
7572.8301	7572.8333	-0.0032	2	2	0	3	4	1	1	1	2	3
7572.7469	7572.744	0.0029	2	2	0	1	2	1	1	1	0	1
7572.6138	7572.6208	-0.007	2	2	0	3	2	1	1	1	1	1
7845.5661	7845.5687	-0.0026	6	1	6	7	8	5	0	5	6	7
7845.4719	7845.4709	0.001	6	1	6	7	7	5	0	5	6	6
2724.4095	2724.4079	0.0016	4	1	3	5	4	4	0	4	5	4

Table S29: List of lines assigned for the C6 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2237.4211	2237.4098	0.0113	3	1	2	3	3	3	0	3	3	3
2237.1754	2237.1889	-0.0135	3	1	2	2	2	3	0	3	2	2
2236.5502	2236.5375	0.0127	3	1	2	4	3	3	0	3	4	3
2236.4369	2236.4477	-0.0108	3	1	2	2	1	3	0	3	2	1
2531.1956	2531.1961	-0.0005	3	0	3	3	2	2	1	2	2	1
2531.1059	2531.1057	0.0002	3	0	3	4	4	2	1	2	3	3
2531.0213	2531.0273	-0.006	3	0	3	3	3	2	1	2	2	2
2530.8934	2530.8943	-0.0009	3	0	3	3	3	2	1	2	3	3
2728.609	2728.6059	0.0031	4	1	3	4	3	4	0	4	4	3
2728.5296	2728.5337	-0.0041	4	1	3	5	6	4	0	4	5	6
2728.4283	2728.4198	0.0085	4	1	3	5	4	4	0	4	5	4
2728.3644	2728.356	0.0084	4	1	3	3	2	4	0	4	3	2
2729.013	2729.0192	-0.0062	4	1	3	5	5	4	0	4	5	5
2829.2431	2829.2293	0.0138	1	1	1	1	1	0	0	0	1	2
2829.4593	2829.4581	0.0012	1	1	1	2	3	0	0	0	1	2
2829.6086	2829.6071	0.0015	1	1	1	2	2	0	0	0	1	2
3956.0177	3956.0157	0.002	2	1	2	2	1	1	0	1	2	1
3956.1021	3956.1091	-0.007	2	1	2	3	2	1	0	1	2	1
3956.887	3956.8965	-0.0095	2	1	2	3	4	1	0	1	2	3
3957.0293	3957.033	-0.0037	2	1	2	3	3	1	0	1	2	2
3957.2309	3957.2308	0.0001	2	1	2	1	1	1	0	1	1	0

3979.4302	3979.4307	-0.0005	4	0	4	5	6	3	1	3	4	5
3979.3799	3979.3747	0.0052	4	0	4	5	4	3	1	3	4	3
4021.2753	4021.2715	0.0038	6	2	4	7	7	6	1	5	7	7
4021.1609	4021.1502	0.0107	6	2	4	6	7	6	1	5	6	7
4021.0927	4021.0969	-0.0042	6	2	4	7	8	6	1	5	7	8
4032.9564	4032.9569	-0.0005	5	2	3	6	7	5	1	4	6	7
4033.1484	4033.144	0.0044	5	2	3	6	6	5	1	4	6	6
4163.3544	4163.3431	0.0113	4	2	2	5	5	4	1	3	5	5
4163.0959	4163.0877	0.0082	4	2	2	5	6	4	1	3	5	6
4358.6929	4358.6953	-0.0024	3	2	1	3	4	3	1	2	3	4
4358.6191	4358.6151	0.004	3	2	1	4	5	3	1	2	4	5
4358.451	4358.4636	-0.0126	3	2	1	4	3	3	1	2	4	3
4359.081	4359.0707	0.0103	3	2	1	4	4	3	1	2	4	4
4778.3934	4778.3972	-0.0038	6	1	5	7	8	5	2	4	6	7
4778.3166	4778.3158	0.0008	6	1	5	7	7	5	2	4	6	6
4997.6435	4997.6453	-0.0018	3	1	3	4	5	2	0	2	3	4
4997.6435	4997.6419	0.0016	3	1	3	2	3	2	0	2	1	2
4997.4934	4997.5017	-0.0083	3	1	3	4	3	2	0	2	3	2
4997.3722	4997.3705	0.0017	3	1	3	3	2	2	0	2	2	1
5105.1153	5105.1167	-0.0014	2	2	1	3	2	2	1	2	3	2
5105.0486	5105.0559	-0.0073	2	2	1	1	0	2	1	2	2	1
5105.0486	5105.0531	-0.0045	2	2	1	2	1	2	1	2	1	0
5105.2088	5105.2115	-0.0027	2	2	1	2	1	2	1	2	3	2
5105.707	5105.7084	-0.0014	2	2	1	1	2	2	1	2	1	2
5105.8767	5105.8786	-0.0019	2	2	1	3	4	2	1	2	3	4
5106.2751	5106.2805	-0.0054	2	2	1	2	3	2	1	2	2	3
5107.3024	5107.3112	-0.0088	2	2	1	1	1	2	1	2	1	1
5107.4069	5107.4103	-0.0034	2	2	1	3	3	2	1	2	3	3
5107.6632	5107.6696	-0.0064	2	2	1	2	2	2	1	2	2	2
5107.538	5107.5366	0.0014	2	2	1	2	2	2	1	2	3	3
5394.5693	5394.569	0.0003	3	2	2	2	1	3	1	3	2	1
5394.7002	5394.6974	0.0028	3	2	2	4	3	3	1	3	4	3
5394.9135	5394.907	0.0065	3	2	2	2	3	3	1	3	2	3
5394.9945	5394.991	0.0035	3	2	2	4	5	3	1	3	4	5
5395.2741	5395.2781	-0.004	3	2	2	3	4	3	1	3	3	4
5395.8325	5395.8374	-0.0049	3	2	2	2	2	3	1	3	2	2
5395.9143	5395.9096	0.0047	3	2	2	4	4	3	1	3	4	4
5396.1491	5396.1523	-0.0032	3	2	2	3	3	3	1	3	3	3
5784.5253	5784.5177	0.0076	4	2	3	5	4	4	1	4	5	4
5784.4486	5784.4443	0.0043	4	2	3	3	2	4	1	4	3	2
5784.9176	5784.9144	0.0032	4	2	3	4	5	4	1	4	4	5
5785.346	5785.3499	-0.0039	4	2	3	5	5	4	1	4	5	5

5785.5663	5785.5661	0.0002	4	2	3	4	4	4	1	4	4	4
5972.743	5972.7466	-0.0036	4	1	4	5	6	3	0	3	4	5
5972.5609	5972.5519	0.009	4	1	4	4	4	3	0	3	3	3
6276.4796	6276.4755	0.0041	5	2	4	5	4	5	1	5	5	4
6276.5967	6276.5922	0.0045	5	2	4	5	6	5	1	5	5	6
6276.9317	6276.9304	0.0013	5	2	4	6	6	5	1	5	6	6
6277.1361	6277.1293	0.0068	5	2	4	5	5	5	1	5	5	5
6276.3811	6276.3818	-0.0007	5	2	4	6	7	5	1	5	6	7
6276.2749	6276.277	-0.0021	5	2	4	6	5	5	1	5	6	5
6913.2841	6913.2781	0.006	5	1	5	6	7	4	0	4	5	6
6913.0871	6913.0898	-0.0027	5	1	5	5	5	4	0	4	4	4
6913.1647	6913.1691	-0.0044	5	1	5	6	6	4	0	4	5	5
7360.9836	7360.9731	0.0105	2	2	1	3	4	1	1	0	2	3
7361.1401	7361.1373	0.0028	2	2	1	3	3	1	1	0	2	2
7361.8227	7361.8176	0.0051	2	2	1	3	3	1	1	0	2	3
7361.2527	7361.2636	-0.0109	2	2	1	2	2	1	1	0	2	2
7563.1746	7563.1782	-0.0036	2	2	0	3	4	1	1	1	2	3
7563.3867	7563.395	-0.0083	2	2	0	2	3	1	1	1	1	2
7562.958	7562.97	-0.012	2	2	0	3	2	1	1	1	1	1
7563.0898	7563.0873	0.0025	2	2	0	1	2	1	1	1	0	1
7564.0311	7564.0285	0.0026	2	2	0	2	2	1	1	1	2	1
7564.18	7564.1899	-0.0099	2	2	0	2	2	1	1	1	1	2
7562.5886	7562.5922	-0.0036	2	2	0	3	2	1	1	1	2	2
7562.8003	7562.8071	-0.0068	2	2	0	1	0	1	1	1	1	1
7562.695	7562.6919	0.0031	2	2	0	2	1	1	1	1	2	2
7853.0208	7853.013	0.0078	6	1	6	7	8	5	0	5	6	7
7852.8626	7852.8535	0.0091	6	1	6	6	6	5	0	5	5	5

Table S30: List of lines assigned for the N11 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	F'	J	K_a	K_c	F
2233.2559	2233.2489	0.007	3	1	2	4	3	0	3	4
2233.0717	2233.0663	0.0054	3	1	2	2	3	0	3	2
2233.775	2233.7708	0.0042	3	1	2	3	3	0	3	3
2502.4081	2502.4019	0.0062	3	0	3	4	2	1	2	3
2502.1684	2502.1592	0.0092	3	0	3	3	2	1	2	2
2718.2695	2718.2654	0.0041	4	1	3	4	4	0	4	4
2717.7901	2717.784	0.0061	4	1	3	5	4	0	4	5
2717.6694	2717.6603	0.0091	4	1	3	3	4	0	4	3
2827.9318	2827.9265	0.0053	1	1	1	1	0	0	0	1

2827.7925	2827.7863	0.0062	1	1	1	2	0	0	0	1
2958.5234	2958.5309	-0.0075	5	1	4	6	4	2	3	5
2958.3311	2958.3267	0.0044	5	1	4	5	4	2	3	4
3384.9684	3384.9613	0.0071	5	1	4	5	5	0	5	5
3384.4922	3384.4843	0.0079	5	1	4	6	5	0	5	6
3384.3961	3384.3872	0.0089	5	1	4	4	5	0	5	4
3943.23	3943.2223	0.0077	4	0	4	5	3	1	3	4
3943.1563	3943.152	0.0043	4	0	4	4	3	1	3	3
3949.7856	3949.7796	0.006	2	1	2	3	1	0	1	2
3949.8798	3949.8766	0.0032	2	1	2	2	1	0	1	1
4049.0917	4049.0901	0.0016	5	2	3	5	5	1	4	5
4181.9958	4181.9962	-0.0004	4	2	2	4	4	1	3	4
4181.7562	4181.7517	0.0045	4	2	2	5	4	1	3	5
4181.684	4181.6888	-0.0048	4	2	2	3	4	1	3	3
4243.4964	4243.499	-0.0026	6	1	5	6	6	0	6	6
4243.0194	4243.0186	0.0008	6	1	5	7	6	0	6	7
4242.933	4242.9376	-0.0046	6	1	5	5	6	0	6	5
4377.4121	4377.4113	0.0008	3	2	1	4	3	1	2	4
4377.2565	4377.2591	-0.0026	3	2	1	2	3	1	2	2
4377.8553	4377.8464	0.0089	3	2	1	3	3	1	2	3
4501.6627	4501.6738	-0.0111	8	2	6	8	8	1	7	8
4501.4616	4501.4625	-0.0009	8	2	6	9	8	1	7	9
4701.7259	4701.7316	-0.0057	6	1	5	7	5	2	4	6
4986.0204	4986.0136	0.0068	3	1	3	4	2	0	2	3
4985.8599	4985.8662	-0.0063	3	1	3	2	2	0	2	1
5787.6758	5787.68	-0.0042	4	2	3	5	4	1	4	5
5787.5098	5787.51	-0.0002	4	2	3	3	4	1	4	3
5956.9759	5956.9734	0.0025	4	1	4	5	3	0	3	4
6273.3204	6273.3264	-0.006	5	2	4	6	5	1	5	6
6273.8745	6273.8715	0.003	5	2	4	5	5	1	5	5
6273.2094	6273.2155	-0.0061	5	2	4	4	5	1	5	4
6732.0313	6732.0394	-0.0081	6	0	6	7	5	1	5	6
6893.0042	6893.0021	0.0021	5	1	5	6	4	0	4	5
7361.3959	7361.4021	-0.0062	2	2	1	3	1	1	0	2
7362.2062	7362.2042	0.002	2	2	1	2	1	1	0	2
7561.7146	7561.7193	-0.0047	2	2	0	2	1	1	1	1
7561.8556	7561.8595	-0.0039	2	2	0	2	1	1	1	2
7561.0286	7561.0329	-0.0043	2	2	0	3	1	1	1	2
7560.7798	7560.7843	-0.0045	2	2	0	1	1	1	1	0
7560.4374	7560.4335	0.0039	2	2	0	1	1	1	1	1
7827.201	7827.2035	-0.0025	6	1	6	6	5	0	5	5
7827.3071	7827.3062	0.0009	6	1	6	7	5	0	5	6

6859.2208	6859.2186	0.0022	6	2	5	7	6	1	6	7
5956.8675	5956.8603	0.0072	4	1	4	4	3	0	3	3
6859.146	6859.138	0.008	6	2	5	5	6	1	6	5
7541.9852	7541.9936	-0.0084	7	2	6	6	7	1	7	6
7542.0556	7542.0562	-0.0006	7	2	6	8	7	1	7	8
6892.8799	6892.8845	-0.0046	5	1	5	5	4	0	4	4
7542.4915	7542.4907	0.0008	7	2	6	7	7	1	7	7
6728.222	6728.2135	0.0085	8	3	5	8	8	2	6	8
6728.15	6728.1527	-0.0027	8	3	5	9	8	2	6	9
7361.5921	7361.5961	-0.004	2	2	1	2	1	1	0	1
4985.9492	4985.949	0.0002	3	1	3	3	2	0	2	2
4048.9052	4048.9102	-0.005	5	2	3	6	5	1	4	6

Table S31: List of lines assigned for the O12 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2188.5024	2188.5086	-0.0062	3	1	2	3	4	3	0	3	3	4
2188.2619	2188.2603	0.0016	3	1	2	2	3	3	0	3	2	3
2188.1526	2188.1463	0.0063	3	1	2	4	3	3	0	3	4	3
2188.8489	2188.8569	-0.008	3	1	2	4	4	3	0	3	4	4
2519.1743	2519.1728	0.0015	3	0	3	4	5	2	1	2	3	4
2519.1051	2519.1063	-0.0012	3	0	3	3	4	2	1	2	2	3
2680.8817	2680.8876	-0.0059	4	1	3	5	6	4	0	4	5	6
2681.0787	2681.0802	-0.0015	4	1	3	4	5	4	0	4	4	5
2681.3797	2681.3847	-0.005	4	1	3	5	5	4	0	4	5	5
2763.2006	2763.1973	0.0033	1	1	1	2	3	0	0	0	1	2
2763.3209	2763.324	-0.0031	1	1	1	2	2	0	0	0	1	2
3063.8392	3063.8312	0.008	5	1	4	6	6	4	2	3	5	5
3359.3585	3359.3549	0.0036	5	1	4	6	6	5	0	5	6	6
3359.5501	3359.5444	0.0057	5	1	4	5	5	5	0	5	5	5
4793.4516	4793.4513	0.0003	6	1	5	7	8	5	2	4	6	7
4895.4167	4895.4119	0.0048	3	1	3	4	5	2	0	2	3	4
4895.3469	4895.347	-0.0001	3	1	3	3	4	2	0	2	2	3
4895.2576	4895.2495	0.0081	3	1	3	3	3	2	0	2	2	2
5250.3258	5250.3346	-0.0088	3	2	2	3	4	3	1	3	3	4
5250.0497	5250.0433	0.0064	3	2	2	4	5	3	1	3	4	5
5249.7462	5249.7561	-0.0099	3	2	2	4	3	3	1	3	4	3
5250.8674	5250.8719	-0.0045	3	2	2	2	2	3	1	3	2	2
6692.3443	6692.3407	0.0036	6	0	6	7	8	5	1	5	6	7
7382.2489	7382.258	-0.0091	2	2	0	3	4	1	1	1	2	3

7382.4754	7382.4753	0.0001	2	2	0	2	3	1	1	1	1	2
7382.1677	7382.1678	-0.0001	2	2	0	1	2	1	1	1	0	1
7382.0291	7382.0257	0.0034	2	2	0	3	2	1	1	1	1	1
7981.5336	7981.538	-0.0044	7	0	7	8	9	6	1	6	7	8
3944.2569	3944.2652	-0.0083	4	0	4	4	5	3	1	3	3	4
4793.379	4793.3861	-0.0071	6	1	5	5	5	5	2	4	4	4
2188.325	2188.3168	0.0082	3	1	2	4	5	3	0	3	4	5
2518.8597	2518.8639	-0.0042	3	0	3	3	3	2	1	2	2	2
2681.567	2681.561	0.006	4	1	3	4	4	4	0	4	4	4
3063.9976	3063.9995	-0.0019	5	1	4	5	4	4	2	3	4	3
3358.868	3358.8636	0.0044	5	1	4	6	7	5	0	5	6	7
3872.395	3872.3873	0.0077	2	1	2	3	4	1	0	1	2	3
3872.5045	3872.5056	-0.0011	2	1	2	3	3	1	0	1	2	2
4029.4931	4029.5009	-0.0078	4	2	2	5	6	4	1	3	5	6
5853.5766	5853.5842	-0.0076	4	1	4	4	4	3	0	3	3	3
5853.6749	5853.6667	0.0082	4	1	4	5	5	3	0	3	4	4
7180.448	7180.4374	0.0106	2	2	1	3	4	1	1	0	2	3
3907.4893	3907.4853	0.004	5	2	3	6	7	5	1	4	6	7
3907.6664	3907.6635	0.0029	5	2	3	6	6	5	1	4	6	6

Table S32: List of lines assigned for the O13 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs–Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2222.0722	2222.059	0.0132	3	1	2	4	4	3	0	3	4	4
2221.3755	2221.3654	0.0101	3	1	2	4	3	3	0	3	4	3
2407.003	2406.9954	0.0076	3	0	3	3	3	2	1	2	2	2
2407.0688	2407.0703	-0.0015	3	0	3	4	4	2	1	2	3	3
2407.3028	2407.3059	-0.0031	3	0	3	4	5	2	1	2	3	4
2682.5249	2682.5288	-0.0039	4	1	3	5	4	4	0	4	5	4
2682.7071	2682.7042	0.0029	4	1	3	4	3	4	0	4	4	3
2683.2933	2683.2961	-0.0028	4	1	3	4	4	4	0	4	4	4
2821.1952	2821.19	0.0052	1	1	1	1	1	0	0	0	1	2
2821.4208	2821.4191	0.0017	1	1	1	2	3	0	0	0	1	2
2821.5693	2821.569	0.0003	1	1	1	2	2	0	0	0	1	2
3823.6381	3823.6269	0.0112	4	0	4	5	6	3	1	3	4	5
3823.5751	3823.5643	0.0108	4	0	4	5	5	3	1	3	4	4
3925.3305	3925.3305	0	2	1	2	3	4	1	0	1	2	3
3925.4728	3925.4671	0.0057	2	1	2	3	3	1	0	1	2	2
3924.5453	3924.5465	-0.0012	2	1	2	3	2	1	0	1	2	1
3924.6512	3924.649	0.0022	2	1	2	3	3	1	0	1	2	3

4100.825	4100.8201	0.0049	5	2	3	6	7	5	1	4	6	7
4241.7155	4241.716	-0.0005	4	2	2	4	5	4	1	3	4	5
5903.6469	5903.6503	-0.0034	4	1	4	5	6	3	0	3	4	5
7876.6492	7876.6565	-0.0073	7	0	7	8	9	6	1	6	7	8
5222.1375	5222.1419	-0.0044	5	0	5	6	6	4	1	4	5	5
5903.5413	5903.5471	-0.0058	4	1	4	5	5	3	0	3	4	4
5903.4687	5903.4584	0.0103	4	1	4	4	4	3	0	3	3	3
4101.0091	4100.9987	0.0104	5	2	3	6	6	5	1	4	6	6
2221.475	2221.4761	-0.0011	3	1	2	2	3	3	0	3	2	3
2221.7231	2221.722	0.0011	3	1	2	3	4	3	0	3	3	4
2222.0131	2222.0106	0.0025	3	1	2	2	2	3	0	3	2	2
2221.5375	2221.5315	0.006	3	1	2	4	5	3	0	3	4	5
4437.0712	4437.0746	-0.0034	3	2	1	4	3	3	1	2	4	3
4437.2245	4437.2247	-0.0002	3	2	1	4	5	3	1	2	4	5
4636.3716	4636.3712	0.0004	2	2	0	2	3	2	1	1	2	3
4636.1	4636.0956	0.0044	2	2	0	1	2	2	1	1	1	2
5222.139	5222.1419	-0.0029	5	0	5	6	6	4	1	4	5	5
5426.7411	5426.7433	-0.0022	3	2	2	3	4	3	1	3	3	4
5427.3766	5427.3803	-0.0037	3	2	2	4	4	3	1	3	4	4
5427.6208	5427.6125	0.0083	3	2	2	3	3	3	1	3	3	3
5903.5422	5903.5471	-0.0049	4	1	4	5	5	3	0	3	4	4
5903.6462	5903.6503	-0.0041	4	1	4	5	6	3	0	3	4	5
7551.5201	7551.5372	-0.0171	2	2	0	3	4	1	1	1	2	3
7552.2416	7552.2518	-0.0102	2	2	0	3	3	1	1	1	2	2
7741.3921	7741.387	0.0051	6	1	6	7	8	5	0	5	6	7
7741.3004	7741.2876	0.0128	6	1	6	7	7	5	0	5	6	6
7814.5454	7814.5469	-0.0015	5	3	2	5	6	5	2	3	5	6
7876.6492	7876.6565	-0.0073	7	0	7	8	9	6	1	6	7	8

Table S33: List of lines assigned for the C14 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	I'_{12}	F'	J	K_a	K_c	I_{12}	F
2229.4795	2229.4733	0.0062	3	1	2	3	3	3	0	3	3	3
2229.3173	2229.3072	0.0101	3	1	2	4	4	3	0	3	4	4
2229.2686	2229.2574	0.0112	3	1	2	2	2	3	0	3	2	2
2228.9751	2228.9715	0.0036	3	1	2	3	4	3	0	3	3	4
2228.7859	2228.7748	0.0111	3	1	2	4	5	3	0	3	4	5
2228.7225	2228.7175	0.005	3	1	2	2	3	3	0	3	2	3
2228.607	2228.6075	-0.0005	3	1	2	4	3	3	0	3	4	3
2228.5264	2228.5197	0.0067	3	1	2	2	1	3	0	3	2	1

2484.3338	2484.3355	-0.0017	3	0	3	4	5	2	1	2	3	4
2484.0878	2484.0937	-0.0059	3	0	3	4	4	2	1	2	3	3
2484.0235	2484.0152	0.0083	3	0	3	3	3	2	1	2	2	2
2483.8884	2483.8842	0.0042	3	0	3	3	3	2	1	2	3	3
2709.6162	2709.6108	0.0054	4	1	3	4	4	4	0	4	4	4
2709.4198	2709.4274	-0.0076	4	1	3	5	5	4	0	4	5	5
2709.1514	2709.146	0.0054	4	1	3	4	5	4	0	4	4	5
2709.0242	2709.0135	0.0107	4	1	3	4	3	4	0	4	4	3
2708.9342	2708.9455	-0.0113	4	1	3	5	6	4	0	4	5	6
2708.7734	2708.77	0.0034	4	1	3	3	2	4	0	4	3	2
2708.8419	2708.8322	0.0097	4	1	3	5	4	4	0	4	5	4
2823.3774	2823.3704	0.007	1	1	1	1	1	0	0	0	1	2
2823.6065	2823.6056	0.0009	1	1	1	2	3	0	0	0	1	2
2823.7633	2823.7599	0.0034	1	1	1	2	2	0	0	0	1	2
3369.802	3369.7935	0.0085	5	1	4	5	6	5	0	5	5	6
3369.5959	3369.5827	0.0132	5	1	4	6	7	5	0	5	6	7
3369.4968	3369.4935	0.0033	5	1	4	6	5	5	0	5	6	5
3919.6318	3919.6269	0.0049	4	0	4	5	6	3	1	3	4	5
3940.5799	3940.5698	0.0101	2	1	2	2	1	1	0	1	2	1
3940.6727	3940.6622	0.0105	2	1	2	3	2	1	0	1	2	1
3940.7682	3940.7695	-0.0013	2	1	2	3	3	1	0	1	2	3
3941.6059	3941.5988	0.0071	2	1	2	3	3	1	0	1	2	2
3941.6945	3941.6927	0.0018	2	1	2	1	2	1	0	1	1	2
3941.8017	3941.7959	0.0058	2	1	2	1	1	1	0	1	1	0
3941.4514	3941.4573	-0.0059	2	1	2	3	4	1	0	1	2	3
3942.6331	3942.6244	0.0087	2	1	2	3	2	1	0	1	2	2
4031.6888	4031.6781	0.0107	6	2	4	6	7	6	1	5	6	7
4031.801	4031.7994	0.0016	6	2	4	7	7	6	1	5	7	7
4031.6174	4031.6272	-0.0098	6	2	4	7	8	6	1	5	7	8
4052.7933	4052.7844	0.0089	5	2	3	6	6	5	1	4	6	6
4052.6005	4052.5979	0.0026	5	2	3	6	7	5	1	4	6	7
4186.6994	4186.7017	-0.0023	4	2	2	4	5	4	1	3	4	5
4186.9274	4186.9149	0.0125	4	2	2	5	5	4	1	3	5	5
4186.5968	4186.5942	0.0026	4	2	2	5	4	4	1	3	5	4
4220.885	4220.8768	0.0082	6	1	5	6	7	6	0	6	6	7
4221.1243	4221.1288	-0.0045	6	1	5	7	7	6	0	6	7	7
4382.6427	4382.6439	-0.0012	3	2	1	3	3	3	1	2	3	3
4382.5754	4382.5761	-0.0007	3	2	1	4	4	3	1	2	4	4
4382.1916	4382.1969	-0.0053	3	2	1	3	4	3	1	2	3	4
4382.1164	4382.1156	0.0008	3	2	1	4	5	3	1	2	4	5
4489.758	4489.7511	0.0069	8	2	6	8	8	8	1	7	8	8
4489.6605	4489.6641	-0.0036	8	2	6	9	9	8	1	7	9	9

4489.4589	4489.457	0.0019	8	2	6	9	10	8	1	7	9	10
4585.7632	4585.7712	-0.008	2	2	0	3	3	2	1	1	3	3
4585.9061	4585.9005	0.0056	2	2	0	2	2	2	1	1	2	2
4584.9268	4584.9307	-0.0039	2	2	0	2	3	2	1	1	2	3
4584.7197	4584.729	-0.0093	2	2	0	3	4	2	1	1	3	4
4584.1973	4584.1942	0.0031	2	2	0	3	2	2	1	1	3	2
4974.1225	4974.1227	-0.0002	3	1	3	4	5	2	0	2	3	4
4973.9728	4973.9712	0.0016	3	1	3	3	3	2	0	2	2	2
5248.5334	5248.5397	-0.0063	7	1	6	7	8	7	0	7	7	8
5248.9948	5249.0014	-0.0066	7	1	6	7	7	7	0	7	7	7
5248.4595	5248.4702	-0.0107	7	1	6	7	6	7	0	7	7	6
5248.3181	5248.3166	0.0015	7	1	6	8	9	7	0	7	8	9
5400.0604	5400.0626	-0.0022	3	2	2	2	1	3	1	3	2	1
5400.1881	5400.1894	-0.0013	3	2	2	4	3	3	1	3	4	3
5400.4031	5400.4014	0.0017	3	2	2	2	3	3	1	3	2	3
5400.4863	5400.4841	0.0022	3	2	2	4	5	3	1	3	4	5
5400.7637	5400.7676	-0.0039	3	2	2	3	4	3	1	3	3	4
5401.3315	5401.3335	-0.002	3	2	2	2	2	3	1	3	2	2
5401.4048	5401.4049	-0.0001	3	2	2	4	4	3	1	3	4	4
5782.1844	5782.1848	-0.0004	4	2	3	3	2	4	1	4	3	2
5782.2672	5782.2571	0.0101	4	2	3	5	4	4	1	4	5	4
5782.4155	5782.4175	-0.002	4	2	3	5	6	4	1	4	5	6
5782.6482	5782.6503	-0.0021	4	2	3	4	5	4	1	4	4	5
5783.305	5783.3026	0.0024	4	2	3	4	4	4	1	4	4	4
5941.7832	5941.7818	0.0014	4	1	4	5	6	3	0	3	4	5
6264.4355	6264.4354	0.0001	5	2	4	5	4	5	1	5	5	4
6264.5462	6264.5518	-0.0056	5	2	4	5	6	5	1	5	5	6
6264.8959	6264.8934	0.0025	5	2	4	6	6	5	1	5	6	6
6265.0834	6265.0886	-0.0052	5	2	4	5	5	5	1	5	5	5
6413.0052	6413.0115	-0.0063	9	3	6	10	10	9	2	7	10	10
6699.7331	6699.7398	-0.0067	6	0	6	7	8	5	1	5	6	7
6742.9776	6742.9708	0.0068	8	3	5	9	9	8	2	6	9	9
6742.8982	6742.8939	0.0043	8	3	5	8	9	8	2	6	8	9
6874.1788	6874.178	0.0008	5	1	5	5	5	4	0	4	4	4
6874.2648	6874.2557	0.0091	5	1	5	6	6	4	0	4	5	5
7351.884	7351.8958	-0.0118	2	2	1	3	2	1	1	0	2	2
7352.7675	7352.7731	-0.0056	2	2	1	1	2	1	1	0	1	2
7353.1736	7353.1748	-0.0012	2	2	1	3	3	1	1	0	2	2
7353.3659	7353.363	0.0029	2	2	1	2	2	1	1	0	1	1
7353.488	7353.4829	0.0051	2	2	1	3	2	1	1	0	2	1
7353.5812	7353.5775	0.0037	2	2	1	2	1	1	1	0	2	1
7550.4057	7550.4068	-0.0011	2	2	0	3	2	1	1	1	2	2

7550.7892	7550.7963	-0.0071	2	2	0	3	2	1	1	1	1	1
7550.9124	7550.9119	0.0005	2	2	0	1	2	1	1	1	0	1
7550.9996	7551.0012	-0.0016	2	2	0	3	4	1	1	1	2	3
7551.2094	7551.2148	-0.0054	2	2	0	2	3	1	1	1	1	2
7551.7097	7551.7229	-0.0132	2	2	0	3	3	1	1	1	2	2
7551.8427	7551.8522	-0.0095	2	2	0	2	2	1	1	1	2	1
7804.7342	7804.7416	-0.0074	6	1	6	7	8	5	0	5	6	7
7804.6474	7804.6456	0.0018	6	1	6	7	7	5	0	5	6	6
7804.5842	7804.5827	0.0015	6	1	6	6	6	5	0	5	5	5
7353.0476	7353.0528	-0.0052	2	2	1	2	3	1	1	0	1	2
2484.1847	2484.1896	-0.0049	3	0	3	3	2	2	1	2	2	1
4381.9569	4381.9626	-0.0057	3	2	1	4	3	3	1	2	4	3
6264.3439	6264.3453	-0.0014	5	2	4	6	7	5	1	5	6	7
6264.2421	6264.2405	0.0016	5	2	4	6	5	5	1	5	6	5

Table S34: List of lines assigned for the N15 isotopologue of 3-NBN.

Observed [MHz]	Calculated [MHz]	Obs-Calc [MHz]	J'	K'_a	K'_c	F'	J	K_a	K_c	F
2214.9425	2214.9377	0.0048	3	1	2	3	3	0	3	3
2214.7213	2214.7226	-0.0013	3	1	2	4	3	0	3	4
2688.3448	2688.3432	0.0016	4	1	3	4	4	0	4	4
2688.1397	2688.1308	0.0089	4	1	3	5	4	0	4	5
2688.0772	2688.0762	0.001	4	1	3	3	4	0	4	3
2807.1642	2807.1628	0.0014	1	1	1	2	0	0	0	1
2866.5802	2866.5765	0.0037	5	1	4	6	4	2	3	5
3339.6256	3339.6234	0.0022	5	1	4	5	5	0	5	5
3877.2016	3877.203	-0.0014	4	0	4	5	3	1	3	4
4015.5075	4015.5038	0.0037	6	2	4	7	6	1	5	7
4015.5597	4015.5552	0.0045	6	2	4	6	6	1	5	6
4144.0135	4144.0167	-0.0032	7	2	5	8	7	1	6	8
4144.0893	4144.0859	0.0034	7	2	5	7	7	1	6	7
5095.8182	5095.8204	-0.0022	2	2	1	3	2	1	2	3
5096.2862	5096.2892	-0.003	2	2	1	2	2	1	2	2
5095.5563	5095.5599	-0.0036	2	2	1	1	2	1	2	1
5096.0572	5096.0586	-0.0014	2	2	1	3	2	1	2	2
5375.8608	5375.8663	-0.0055	3	2	2	3	3	1	3	3
5752.5515	5752.5561	-0.0046	4	2	3	3	4	1	4	3
5752.6193	5752.6196	-0.0003	4	2	3	5	4	1	4	5
5752.8705	5752.8664	0.0041	4	2	3	4	4	1	4	4
5899.9344	5899.9372	-0.0028	4	1	4	4	3	0	3	3

5900.0067	5900.0137	-0.007	4	1	4	5	3	0	3	4
6228.4363	6228.439	-0.0027	5	2	4	6	5	1	5	6
6228.6585	6228.6541	0.0044	5	2	4	5	5	1	5	5
6636.0532	6636.0472	0.006	6	0	6	7	5	1	5	6
6824.8946	6824.8907	0.0039	5	1	5	6	4	0	4	5
6824.8134	6824.8201	-0.0067	5	1	5	5	4	0	4	4
7312.9532	7312.9505	0.0027	2	2	1	3	1	1	0	2
7508.4554	7508.4586	-0.0032	2	2	0	3	1	1	1	2
7508.3158	7508.3129	0.0029	2	2	0	1	1	1	1	0
7508.7038	7508.709	-0.0052	2	2	0	2	1	1	1	1
7935.1851	7935.1909	-0.0058	7	0	7	8	6	1	6	7
2453.9595	2453.9676	-0.0081	3	0	3	4	2	1	2	3
3915.509	3915.5082	0.0008	2	1	2	1	1	0	1	0
3916.0514	3916.0463	0.0051	2	1	2	1	1	0	1	1
3915.7093	3915.6987	0.0106	2	1	2	3	1	0	1	2
5375.4537	5375.4469	0.0068	3	2	2	2	3	1	3	2
5095.9168	5095.9186	-0.0018	2	2	1	2	2	1	2	1
4368.9647	4368.9664	-0.0017	3	2	1	4	3	1	2	4
4369.0528	4369.0549	-0.0021	3	2	1	3	3	1	2	3
5279.8118	5279.8072	0.0046	5	0	5	5	4	1	4	4
5375.5591	5375.5557	0.0034	3	2	2	4	3	1	3	4
4039.7072	4039.7032	0.004	5	2	3	6	5	1	4	6
3339.4075	3339.4042	0.0033	5	1	4	6	5	0	5	6
4178.7842	4178.7801	0.0041	6	1	5	7	6	0	6	7
4940.0058	4939.9983	0.0075	3	1	3	3	2	0	2	2
5193.252	5193.2579	-0.0059	7	1	6	8	7	0	7	8
5193.4793	5193.486	-0.0067	7	1	6	7	7	0	7	7
7695.6955	7695.6975	-0.002	5	3	2	6	5	2	3	6
7747.0576	7747.0584	-0.0008	6	1	6	7	5	0	5	6