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Millimeter-Wave Spectrum, Centrifugal Distortion Analysis, and Energy Levels of HNO_3[1]

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One hundred and eleven new rotational transitions of HNO_3 have been measured in the millimeter-microwave region. This data set is the basis for a centrifugal distortion analysis and for the calculation of a complete set of energy levels through $J = 50$. The constants which result from this analysis are (in megahertz): $A = 13\ 011.0287 \pm 0.0057$, $B = 12\ 099.8611 \pm 0.0057$, $C = 6260.6391 \pm 0.0006$, $\Delta_J = (14.038 \pm 0.026) \times 10^{-3}$, $\Delta_{JK} = (-20.1780 \pm 0.0037) \times 10^{-3}$, $\Delta_K = (7.4153 \pm 0.0108) \times 10^{-3}$, $\delta_J = (1.1828 \pm 0.00039) \times 10^{-3}$, $\delta_K = (-20.5648 \pm 0.0046) \times 10^{-3}$, $H_J = (-9.84 \pm 3.82) \times 10^{-8}$, $H_{JK} = (-9.933 \pm 0.367) \times 10^{-8}$, $H_{KJ} = (1.03 \pm 0.12) \times 10^{-7}$, $h_J = (-9.241 \pm 0.127) \times 10^{-9}$, $h_{JK} = (-1.398 \pm 0.032) \times 10^{-7}$, and $h_K = (1.135 \pm 0.027) \times 10^{-6}$.

INTRODUCTION

Nitric acid is a near-oblate asymmetric rotor with rotational constants of the order of 10 GHz and moderate centrifugal distortion. The presence of this species in the atmosphere and its basic role in chemistry have stimulated numerous spectroscopic studies. The rotational spectrum of HNO_3 has been studied in the centimeter-wave region (*1–3*), and Kaushik and Venkateswarlu (*4*) have performed a centrifugal distortion analysis of these data. They noted that the relatively large standard deviations of the resulting coefficients and the indeterminacy of τ_{cccc} must be ascribed to the data set available. Conventional infrared spectroscopy reveals only broad vibrational bands because of the dense rotational fine structure of HNO_3 (*5–8*). Recently, however, Brockman *et al.* (*9*) have published an unassigned diode laser spectrum of HNO_3 in the 11-μm region that clearly resolves the rotational fine structure. Several other diode laser studies of HNO_3 are also in progress (*10*).

In this paper we report the measurement of 111 rotational transitions in the region between 80 and 300 GHz. This spectral coverage results in a well-conditioned data set which makes possible an accurate centrifugal distortion analysis and calculation of energy levels through $J = 50$. These ground-vibrational-state energy levels can serve as a basis for the analysis of the complex rotation–vibration spectra which are now being recorded as well as for the study of

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TABLE I

Observed Microwave Transitions of HNO_3 (MHz)

Transition	Observed frequency	Transition	Observed frequency
1(0 1)- 0(0 0)	18 360.530[a]	10(4 6)- 9(4 5)	181 789.200
1(1 1)- 0(0 0)	19 271.600[a]	11(0 11)-10(1 10)	144 004.240
2(1 2)- 2(1 1)	-17 517.490[a]	11(9 3)-11(9 2)	-12 317.450[a]
2(0 2)- 2(1 1)	-17 616.030[a]	11(3 8)-10(3 7)	181 678.130
2(1 2)- 1(0 1)	31 792.800[a]	12(3 10)-11(2 9)	181 630.790
3(1 2)- 3(3 1)	-22 161.000[a]	12(10 3)-12(10 2)	-9 245.560[a]
3(2 1)- 3(3 0)	-9 447.970[a]	12(1 12)-12(1 11)	-144 339.740
3(1 2)- 3(2 1)	-16 700.740[a]	13(2 12)-12(2 11)	181 594.580
4(3 2)- 4(3 1)	-14 534.250[a]	14(2 12)-14(3 11)	-144 198.890
5(4 2)- 5(4 1)	-12 540.980[a]	14(0 14)-13(1 13)	181 560.280
5(3 3)- 5(3 2)	-29 175.320[a]	14(2 12)-14(4 11)	-144 198.940
6(5 2)- 6(5 1)	-10 344.230[a]	15(1 15)-15(2 14)	-181 995.690
6(4 3)- 6(4 2)	-27 369.670[a]	16(8 9)-16(9 8)	-105 667.150
6(3 4)- 5(3 3)	106 481.320	16(7 9)-16(8 8)	-105 665.850
6(2 4)- 5(2 3)	106 648.550	16(2 15)-16(3 14)	-181 927.420
7(6 2)- 7(6 1)	-8 097.580[a]	17(6 12)-17(7 11)	-143 867.520
7(5 3)- 7(5 2)	-24 993.510[a]	17(2 15)-17(3 14)	-181 848.630
7(1 6)- 6(1 5)	106 483.440	17(3 14)-16(3 13)	256 757.160
8(6 3)- 8(6 2)	-22 147.000[a]	18(4 15)-18(5 14)	-181 758.230
8(7 1)- 7(7 0)	174 944.800	18(6 12)-18(8 11)	-143 715.920
8(7 2)- 7(7 1)	169 702.230	18(2 16)-17(2 15)	256 723.390
8(6 2)- 7(6 1)	180 101.520	19(5 15)-19(6 14)	-181 654.810
8(4 5)- 7(4 4)	144 146.640	19(1 18)-18(1 17)	256 691.080
8(3 5)- 7(3 4)	144 201.860	20(6 15)-20(7 14)	-181 537.330
8(0 8)- 7(0 7)	106 445.510	20(0 20)-19(0 19)	256 657.790
9(7 3)- 9(7 2)	-18 969.560[a]	22(21 1)-22(22 0)	-103 748.090
9(2 7)- 8(2 6)	144 081.990	22(21 2)-22(22 1)	-103 750.640
10(4 6)- 9(5 5)	181 770.440	22(9 14)-22(9 13)	-168 514.480
10(5 6)- 9(4 5)	181 790.820	23(22 1)-23(23 0)	-108 757.340
10(1 9)- 9(2 8)	144 039.780	23(22 2)-23(23 1)	-108 758.550
10(8 3)-10(8 2)	-15 628.190[a]	24(23 1)-24(24 0)	-113 766.890
10(9 1)- 9(9 0)	215 606.940	24(23 2)-24(24 1)	-113 767.610
10(5 6)- 9(5 5)	181 772.040	24(15 9)-24(16 8)	-100 631.670

Transition	Observed frequency	Transition	Observed frequency
25(22 3)-25(23 2)	-100 637.790	34(31 4)-34(32 3)	-146 785.990
25(22 4)-25(23 3)	-100 842.920	34(22 12)-34(24 11)	-135 253.230
25(17 9)-25(18 8)	-100 569.340	35(23 12)-35(25 11)	-134 140.390
25(14 12)-25(15 11)	-141 778.830	35(24 12)-35(24 11)	-133 340.120
25(14 12)-25(14 11)	-141 778.310	36(32 4)-36(33 3)	-147 571.300
26(11 15)-26(13 14)	-180 446.060	36(32 5)-36(33 4)	-147 577.120
27(24 3)-27(25 2)	-111 014.200	36(27 9)-36(29 8)	-141 190.440
27(24 4)-27(25 3)	-111 081.200	36(24 12)-36(26 11)	-132 983.830
28(24 4)-28(25 3)	-105 622.560	36(25 12)-36(25 11)	-131 562.390
28(24 5)-28(25 4)	-106 141.210	37(36 1)-37(37 0)	-179 104.130
30(29 1)-30(30 0)	-143 860.370	37(32 5)-37(33 4)	-142 564.470
30(25 5)-30(26 4)	-103 954.590	37(32 6)-37(33 5)	-142 615.390
30(25 6)-30(26 5)	-105 807.140	37(25 12)-37(27 11)	-131 830.240
30(19 12)-30(20 11)	-138 917.330	37(26 12)-37(26 11)	-129 372.980
30(18 12)-30(19 11)	-138 890.960	38(37 1)-38(38 0)	-184 154.560
30(23 7)-30(25 6)	-144 655.990	38(26 12)-38(28 11)	-130 755.270
30(22 8)-30(24 7)	-108 777.550	38(25 13)-38(27 12)	-145 639.170
30(21 10)-30(21 9)	-107 091.060	38(26 13)-38(26 12)	-145 131.960
30(18 12)-30(20 11)	-138 919.210	38(23 15)-38(25 14)	-174 774.940
30(19 12)-30(19 11)	-138 889.080	38(24 15)-38(24 14)	-174 771.530
30(13 18)-30(13 17)	-217 946.740	38(21 18)-38(21 17)	-215 282.120
31(20 12)-31(21 11)	-138 125.840	38(18 21)-38(18 20)	-254 275.010
31(19 12)-31(20 11)	-138 072.320	40(38 2)-40(39 1)	-185 972.720
31(19 12)-31(21 11)	-138 129.830	40(20 21)-40(20 20)	-253 611.710
31(20 12)-31(20 11)	-138 068.360	42(32 10)-42(34 9)	-182 748.840
32(30 3)-32(31 2)	-145 533.790	43(39 5)-43(40 4)	-183 519.940
32(20 12)-32(22 11)	-137 256.360	44(23 21)-44(24 20)	-251 991.840
32(21 12)-32(21 11)	-137 134.290	45(40 6)-45(41 5)	-184 280.130
33(30 3)-33(31 2)	-141 695.530	46(26 21)-46(26 20)	-251 011.790
33(30 4)-33(31 3)	-141 697.210	47(36 11)-47(38 10)	-212 777.870
33(21 12)-33(23 11)	-136 295.940	48(28 21)-48(28 20)	-249 900.600
33(22 12)-33(22 11)	-136 061.540	50(46 5)-50(47 4)	-219 426.320
34(31 3)-34(32 2)	-146 785.070		

a. See Refs. 1 and 2.

HNO_3 by direct microwave techniques. A preliminary report of this work has been given recently (*11*).

II. EXPERIMENTAL DETAILS

We have previously detailed our general experimental technique (*12*, *13*). A brief description of the specific configuration for this work follows. Millimeter-wave energy was produced by King and Gordy (*14*) crystal harmonic generators driven by OKI klystrons in the 35-GHz range. This energy was focused by quasi-optical techniques through a 4-m-long absorption cell made of 10-cm-diameter KIMAX glass pipe and detected by a 1.6-K InSb photoconduction detector. The HNO_3 vapor was taken directly from a standard laboratory mixture of concentrated nitric acid.

Although most of the lines reported here are strong video oscilloscope lines, source modulation and lock-in techniques were used to record the weaker high-J lines. For this work the 35-GHz klystron was phase locked, via a phased-locked X-13 Varian klystron and transfer oscillator, to a crystal oscillator whose phase was continuously monitored against WWVB.

III. RESULTS AND DISCUSSION

We have used Watson's reduced centrifugal distortion Hamiltonian (*15*) and the computational and statistical techniques that we have previously discussed (*16*, *17*) for the analysis of the rotational spectrum of HNO_3. A "bootstrap" assignment–analysis procedure was used. At each step lines that would provide a balance between a maximum of new, independent information for the analysis and a minimum risk of assignment error were selected for measurement. In practice this amounted to the selection of lines whose prediction uncertainties were several megahertz. This procedure was iterated until all of the approximately 5000 lines of significant strength below $J = 50$ were predicted with an uncertainty of 1 MHz or less.

Table I shows the 131 rotational transitions included in our analysis and Table II shows the spectral constants which result. In our analysis H_K was found to be only marginally determined and was subsequently eliminated from the constant set. The rms deviation of the analysis was 0.124 MHz with or without

TABLE II

Spectroscopic Constants of HNO_3 (MHz)

$A = 13\,011.0287 \pm 0.0057$	$B = 12\,099.8611 \pm 0.0057$	$C = 6\,260.6391 \pm 0.0006$
$\Delta_J = (14.038 \pm 0.026) \cdot 10^{-3}$	$\Delta_{JK} = (-20.1780 \pm 0.0037) \cdot 10^{-3}$	$\Delta_K = (7.4153 \pm 0.0108) \cdot 10^{-3}$
	$\delta_J = (1.1828 \pm 0.00039) \cdot 10^{-3}$	$\delta_K = (-20.5648 \pm 0.0046) \cdot 10^{-3}$
$H_J = (-9.84 \pm 3.82) \cdot 10^{-8}$	$H_{JK} = (-9.933 \pm 0.367) \cdot 10^{-8}$	$H_{KJ} = (1.03 \pm 0.12) \cdot 10^{-7}$
$h_J = (-9.241 \pm 0.127) \cdot 10^{-9}$	$h_{JK} = (-1.398 \pm 0.032) \cdot 10^{-7}$	$h_K = (1.135 \pm 0.027) \cdot 10^{-6}$

TABLE III

Energy Levels of HNO_3 (cm^{-1})

J= 1	0.837507	0.642832	0.612441							
J= 2	2.516096	2.248429	2.257255	1.672934	1.669643					
J= 3	5.041769	4.908752	4.726621	4.185727	4.169544	3.133938	3.133714			
J= 4	8.422871	8.225816	8.023434	7.538624	7.491669	6.478352	6.476797	5.013942	5.013929	
J= 5	12.667310 7.311672	12.601861	12.152971	11.733748	11.630764	10.657081	10.650942	9.194574	9.194461	7.311673
J= 6	17.783357 12.328878	17.736272 10.027046	17.118729 10.027046	16.773683	16.582349	15.669893	15.651903	14.208918	14.208358	12.328885
J= 7	23.764091 18.179599	23.725261 15.880789	22.931486 15.880789	22.661330 13.160053	22.350913 13.160053	21.517220	21.473954	20.055866	20.053836	18.180032
J= 8	30.618468 24.863899	30.604232 22.568646	29.599622 22.568643	29.400315 19.850272	28.939026 19.850272	28.200280 16.710689	28.110601 16.710689	26.734396	26.728415	24.864079
J= 9	38.342729 32.379257	38.334767 30.099754	37.131911 30.099740	36.992798 27.374699	36.353828 27.374699	35.721072 24.237338	35.556339 24.237338	34.243766 20.678945	34.228630 20.678945	32.379882
J= 10	46.626026 40.724387 25.064912	46.621471 33.443141	45.534599 33.443087	45.442768 35.732597	44.603583 35.732596	44.082283 32.598234	43.808766 32.598234	42.583721 29.041987	42.549760 29.041987	40.726232 25.064812
J= 11	56.396605 49.897130 34.264210	56.395353 47.627726 30.888280	54.810485 47.627542 33.388280	54.752607 44.923143	53.697983 44.923139	53.287121 41.792724	52.969660 41.792724	51.754681 38.239273	51.685821 38.239273	49.901946 34.264210

J= 12									
64.727214	64.726824	64.259654	64.224513	63.647507	63.239109	62.744470	61.757852	61.630233	59.905989
59.894629	57.642228	57.641734	54.945421	54.945405	51.820085	51.820085	48.270210	48.270210	44.297821
44.297821	39.993658	39.993658	35.083336	35.083336					
J= 13									
77.924391	77.923742	75.930871	75.960158	74.461941	74.241853	73.441211	72.595253	72.377420	70.737642
70.713051	68.485698	68.484249	65.798423	65.798370	62.679525	62.679524	59.134147	59.134147	55.165094
55.165094	50.773874	50.773874	45.961337	45.961337	40.727966	40.727966			
J= 14									
89.988321	89.988435	87.872638	87.860716	86.148477	85.998816	84.969656	84.269641	83.924868	82.396683
82.347354	80.156566	80.153028	77.481049	77.480893	74.370177	74.370172	70.830377	70.830377	66.885428
66.865423	62.477288	62.477288	57.667423	57.667423	52.436214	52.436214	46.784158	46.784158	
J= 15									
102.920344	102.920172	100.633667	100.626937	98.710624	98.613116	97.340874	96.784356	96.274415	94.883554
94.791304	92.653721	92.645710	89.992108	89.991688	86.891094	86.891079	83.358129	83.358128	79.398177
79.398177	75.013678	75.013678	70.207096	70.207096	64.978455	64.978455	59.328611	59.328611	53.257893
53.257893									
J= 16									
116.718775	116.718687	114.262988	114.259249	112.148670	112.087379	110.566531	110.143111	109.432042	108.199481
108.033120	105.976120	105.959163	103.330334	103.329231	100.241250	100.241207	96.716571	96.716570	92.762640
92.762640	88.383039	88.383039	83.579820	83.579820	78.354208	78.354208	72.706954	72.706954	66.638513
66.638513	60.149156	60.149156							
J= 17									
131.383235	131.383091	128.750896	128.757847	126.461081	126.423669	124.657483	124.349757	123.406764	122.346505
122.081966	120.123091	120.089273	117.494411	117.491946	114.419537	114.419418	110.904806	110.904802	106.958065
106.958065	102.583920	102.583920	97.785022	97.785022	92.562959	92.562959	86.918714	86.918714	80.852901
80.852901	74.365898	74.365898	67.457928	67.457928					
J= 18									
146.915649	146.915627	144.123879	144.122770	141.645788	141.623492	139.621929	139.408040	138.209597	137.327429
136.920153	134.004401	134.000722	132.483024	132.477590	129.424760	129.424456	125.921868	125.921856	121.983647
121.983647	117.615930	117.615930	112.822091	112.822091	107.604157	107.604157	101.963393	101.963393	95.900597
95.900597	89.416277	89.416277	82.510748	82.510748	75.184189	75.184189			
J= 19									
163.213725	163.213724	160.354547	160.353952	157.700385	.687859	155.464159	155.321388	153.852863	153.145683
152.554305	150.890519	150.777021	148.284939	148.283598	.255648	145.254918	141.766716	141.766683	137.838523
137.838522	133.478329	133.478329	128.690375	128.690375	.477219	123.477219	117.840456	117.840456	111.781109
111.781109	105.299836	105.299836	98.397060	98.397060	073039	91.073039	83.327919	83.327919	
J= 20									
180.578007	180.578002	177.451500	177.451264	174.624361	617378	172.184753	172.092745	170.349394	169.805113
168.990737	167.512666	167.321128	164.929116	164.920606	910863	161.909203	158.438236	158.438151	154.521771
154.521768	150.170325	150.170325	145.389183	145.389183	181525	140.181525	134.549342	134.549342	128.493918
128.493918	122.016091	122.016091	115.116410	115.116410	795225	107.795225	100.052749	100.052749	91.889094
91.889094									

TABLE III—*Continued*

J=	21									
	198.708270	198.708267	195.414702	195.414536	192.416591	.412353	189.782134	189.724479	187.711162	187.309754
	186.239227	184.969913	184.656918	132.384852	182.342256	.389035	179.385444	175.935234	175.935024	172.032407
	172.032398	167.691086	167.691085	162.917782	162.917782	.716419	157.716419	152.089454	152.089454	146.038475
	146.038475	139.564532	139.564532	132.668319	132.668319	.350293	125.350293	117.610747	117.610747	109.449851
	109.449851	100.867690	100.867690							
J=	22									
	217.704320	217.704319	214.243656	214.243569	211.075244	1.072875	208.253622	208.218364	205.947422	205.663573
	204.311861	203.244085	202.781238	200.661946	200.584973	7.688804	197.681387	194.256437	194.255947	190.369378
	190.369354	186.039719	186.039713	181.275396	181.275396	5.081209	176.081209	170.460163	170.460163	164.414203
	164.414203	157.944620	157.944620	151.052282	151.052282	3.737768	143.737768	136.001460	136.001460	127.843599
	127.843599	119.264321	119.264321	110.263683	110.263683					
J=	23									
	237.565945	237.565944	233.938193	233.938148	230.600199	10.598882	227.596761	227.575626	225.063334	224.870249
	223.222127	222.359678	221.695563	219.760850	219.628008	16.908905	216.794229	213.400501	213.399409	209.531563
	209.531504	205.215280	205.215277	200.461203	200.461203	95.275165	195.275165	189.660807	189.660807	183.620491
	183.620491	177.155791	177.155791	170.267768	170.267768	62.957146	162.957146	155.224410	155.224410	147.069881
	147.069881	138.493752	138.493752	129.496129	129.496129	20.077045	120.077045			
J=	24									
	258.292922	258.292922	254.498066	254.498043	250.990963	250.990246	247.809484	247.797030	245.059964	244.932990
	242.984011	242.313649	241.406314	239.682794	239.464023	236.748279	236.720404	233.366023	233.363694	229.517768
	229.517626	225.216767	225.216760	220.474338	220.474338	215.297516	215.297516	209.690690	209.690690	203.656702
	203.656702	197.197449	197.197449	190.314220	190.314220	183.007901	183.007901	175.279097	175.279097	167.128217
	167.128217	158.555524	158.555524	149.561175	149.561175	140.145246	140.145246	130.307746	130.307746	
J=	25									
	279.885019	279.885019	275.923024	275.923012	272.247128	272.246739	268.890207	268.882977	265.935571	265.854424
	263.610620	263.110178	261.923850	260.429836	260.086522	257.506207	257.455321	254.151575	254.146801	250.326719
	250.326357	246.043115	246.043099	241.313884	241.313884	236.147454	236.147454	230.549081	230.549081	224.522165
	224.522165	218.068974	218.068974	211.191057	211.191057	203.889484	203.889484	196.164998	196.164998	188.018108
	188.018108	179.449155	179.449155	170.458358	170.458358	161.045836	161.045836	151.211640	151.211640	140.955758
	140.955758									
J=	26									
	302.241996	302.241996	298.212812	298.212806	294.368332	294.368123	290.837746	290.833603	287.687195	287.636558
	285.112316	284.753426	283.261201	282.004833	281.491922	279.082474	278.993164	275.755750	275.746324	271.957071
	271.956365	267.693193	267.693155	262.978875	262.978873	257.824125	257.824125	252.235212	252.235212	246.216176
	246.216176	239.769713	239.769713	232.897666	232.897666	225.601318	225.601318	217.881564	217.881564	209.739029
	209.739029	201.174144	201.174144	192.187191	192.187191	182.778347	182.778347	172.947701	172.947701	162.695277
	162.695277	152.021047	152.021047							
J=	27									
	325.663601	325.663601	321.267165	321.267161	317.354240	317.354128	313.651205	313.648858	310.311780	310.280811
	307.496189	307.247283	305.432955	304.411330	303.681363	301.477518	301.326913	298.177246	298.159289	294.407408
	294.405918	290.165808	290.165715	285.468288	285.468283	280.326634	280.326634	274.748279	274.748279	268.738001
	268.738001	262.258586	262.258586	255.433413	255.433413	248.142802	248.142802	240.428225	240.428225	232.290436
	232.290436	223.729964	223.729964	214.747170	214.747170	205.342287	205.342287	195.515454	195.515454	185.266732
	185.266732	174.596123	174.596123	163.503580	163.503580					

J= 28

349.849572	349.849572	345.385811	345.385810	341.204529	341.204469	337.329889	337.328574	333.806705	333.788089
330.760858	330.595208	328.454240	327.653374	326.661270	324.692557	324.448917	321.414970	321.381933	317.676263
311.673225	313.456680	313.459472	308.781045	308.781034	303.654038	303.654038	298.087437	298.087437	292.086871
292.086871	285.656081	285.656081	278.797631	278.797631	271.513310	271.513310	263.804386	263.804386	255.671760
255.671760	247.116072	247.116072	238.137767	238.137767	228.737147	228.737147	218.914404	218.914404	208.669640
208.669640	198.002893	198.002893	186.914141	186.914141	175.403321	175.403321			

J= 29

374.899638	374.899638	370.268471	370.268471	365.918880	365.918849	361.873230	361.872500	358.169907	358.158882
354.907546	354.660046	352.339311	351.735280	350.442464	348.729642	348.352279	345.468176	345.409445	341.762145
341.756156	327.573465	337.573014	332.916005	332.915979	327.805348	327.805347	322.251804	322.251804	316.261981
316.261981	309.840258	309.840258	302.989628	302.989628	295.712188	295.712188	288.009426	288.009426	279.882408
279.882408	271.331897	271.331897	262.358435	262.358435	252.962398	252.962398	243.144036	243.144036	232.903500
232.903500	222.240965	222.240965	211.156142	211.156142	199.649292	199.649292	187.720233	187.720233	

J= 30

400.813519	400.813519	396.014855	396.014854	391.496977	391.496960	387.280741	387.280340	383.399813	383.393371
379.932269	379.864021	377.099665	376.661376	375.038816	373.591647	373.032948	370.336625	370.235767	366.663597
366.652160	362.502742	362.504798	357.871962	357.871902	352.779521	352.779518	347.240454	347.240454	341.262492
341.262492	334.850741	334.850741	328.008683	328.008683	320.738758	320.738758	313.042702	313.042702	304.921765
304.921765	296.376850	296.376850	287.408604	287.408604	278.017487	278.017487	268.203815	268.203815	257.967791
257.967791	247.309533	247.309533	236.229086	236.229086	224.726439	224.726439	212.801535	212.801535	200.454276
200.454276									

J= 31

427.590922	427.590922	422.624663	422.624663	417.938495	417.938487	413.551983	413.551764	409.495232	409.491512
405.831154	405.738730	402.742380	402.435758	400.465958	399.282161	398.491676	396.020731	395.853608	392.379268
382.358096	388.255224	388.253128	383.647641	383.647503	378.575461	378.575454	373.052418	373.052418	367.087528
367.087528	360.686724	360.686724	353.854043	353.854043	346.592312	346.592312	338.903543	338.903543	330.789193
330.789193	322.250317	322.250317	313.287683	313.287683	303.901843	303.901843	294.093185	294.093185	283.861972
283.861972	273.208367	273.208367	262.132455	262.132455	250.634256	250.634256	238.713738	238.713738	226.370826
226.370826	213.605408	213.605408							

J= 32

455.231546	455.231546	450.097586	450.097586	445.243107	445.243103	440.686545	440.686426	436.455237	436.453112
432.601133	432.575214	429.269703	429.262084	426.740145	425.805314	424.734787	422.521691	422.254986	418.908025
418.370005	414.016775	414.016000	410.241692	410.241406	405.191914	405.191997	399.686681	399.686680	393.736173
393.736173	387.347368	387.347368	380.524929	380.524929	373.272116	373.272116	365.591255	365.591255	357.484027
357.484027	348.951663	348.951663	339.995060	339.995060	330.614874	330.614874	320.811573	320.811573	310.585484
310.585484	299.936823	299.936823	288.865716	288.865716	277.372219	277.372219	265.456329	265.456329	253.117994
253.117994	240.457121	240.457121	227.173585	227.173585					

J= 33

482.735078	482.735078	478.433306	478.433306	473.410479	473.410476	468.684030	468.683966	464.279081	464.277879
460.239547	460.224049	456.680113	456.543427	453.876793	453.165540	451.773480	449.841551	449.432588	446.249086
446.182864	442.199441	442.191218	437.652691	437.652097	432.627963	432.627925	427.142178	427.142176	421.207472
421.207471	414.831797	414.831797	408.020527	408.020527	400.777409	400.777409	393.105114	393.105114	385.005580
385.005580	376.480227	376.480227	367.539099	367.539099	358.155964	358.155964	348.358380	348.358380	338.137745
338.137745	327.494332	327.494332	316.428315	316.428315	304.939786	304.939786	293.028774	293.028774	280.695254
280.695254	267.939157	267.939157	254.760373	254.760373	241.158763	241.158763			

J= 34

513.101198	513.101198	507.631495	507.631495	502.440265	502.440264	497.544048	497.544014	492.966133	492.965459
488.744721	488.735459	484.970079	484.882207	481.888548	481.367325	479.622381	477.983195	477.381875	474.402179
474.260369	470.289506	470.276063	465.879142	465.877941	460.882026	460.881941	455.417793	455.417788	449.500425
449.500425	443.139100	443.139100	436.339994	436.339994	429.107398	429.107398	421.444374	421.444374	413.353140
413.353140	404.835329	404.835329	395.892144	395.892144	386.524479	386.524479	376.732992	376.732992	366.518157
366.518157	355.880311	355.880311	344.819678	344.819678	333.336394	333.336394	321.430522	321.430522	309.102066
309.102066	296.350980	296.350980	283.177177	283.177177	269.580532	269.580532	255.560892	255.560892	

TABLE III—*Continued*

J= 35									
542.325571	543.325571	537.691812	537.691812	532.332116	532.332116	527.266211	527.266193	522.515837	522.515462
518.114841	518.109408	514.135550	514.080190	510.783511	510.414949	508.298125	506.950254	506.103174	503.367688
503.184945	499.361564	499.367227	494.919435	494.917120	489.952848	489.952669	484.512355	484.512344	478.613993
478.613992	472.268331	472.268331	465.482452	465.482452	458.261264	458.261264	450.608258	450.608258	442.525968
442.525968	434.016258	434.016258	425.080513	425.080513	415.719762	415.719762	405.934769	405.934769	395.726098
395.726098	385.094153	385.094153	374.039215	374.039215	362.561465	362.561465	350.661005	350.661005	338.337870
338.337870	325.592041	325.592041	312.423452	312.423452	298.831999	298.831999	284.817545	284.817545	270.379922
270.379922									
J= 36									
574.419856	574.419856	568.613909	568.613909	563.085670	563.085670	557.850127	557.850118	552.927681	552.927475
548.348930	548.345477	544.172821	544.138543	540.564619	540.312271	537.818084	536.746932	535.602666	533.146788
532.858281	529.203436	529.160561	524.772110	524.767575	519.839004	519.838632	514.424633	514.424608	508.547085
508.547083	502.218501	502.218501	495.446992	495.446992	488.238156	488.238156	480.595964	480.595964	472.523300
472.523300	464.022287	464.022287	455.094503	455.094503	445.741131	445.741131	435.963054	435.963054	425.760928
425.760928	415.135233	415.135233	404.086313	404.086313	392.614398	392.614398	380.719633	380.719633	368.402086
368.402086	355.661769	355.661769	342.498638	342.498638	328.912612	328.912612	314.903570	314.903570	300.471359
300.471359	285.615801	285.615801							
J= 37									
606.371697	606.371697	600.397427	600.397427	594.700557	594.700557	589.295401	589.295396	584.201182	584.201069
579.443832	579.443832	575.057930	575.057930	571.230582	571.062567	568.198835	567.377779	565.891840	563.741516
563.302628	559.224269	559.179821	555.435387	555.426922	550.538991	550.538241	545.153334	545.153281	539.298563
539.298559	532.988582	532.988582	526.232667	526.232667	519.037190	519.037190	511.406660	511.406660	503.344347
503.344347	494.859658	494.859658	485.933389	485.933389	476.587887	476.587887	466.817165	466.817165	456.621984
456.621984	446.002906	446.002906	434.960341	434.960341	423.494576	423.494576	411.605800	411.605800	399.294120
399.294120	386.559577	386.559577	373.402157	373.402157	359.821798	359.821798	345.818401	345.818401	331.391828
331.391829	316.541916	316.541916	301.268472	301.268472					
J= 38									
639.184732	639.184732	633.041995	633.041995	627.176398	627.176398	621.601631	621.601628	616.335870	616.335809
611.403762	611.403762	606.851193	606.838615	602.777681	602.668447	599.454186	598.847429	596.986022	595.154766
594.512953	591.253633	591.131453	586.907764	586.892310	582.051235	582.049759	576.697098	576.696986	570.867235
570.867229	564.577503	564.577503	557.838495	557.838495	550.657453	550.657453	543.039486	543.039486	534.988291
534.988291	526.526591	526.526591	517.596419	517.596419	508.259303	508.259303	498.496401	498.496401	488.308584
488.308584	477.696506	477.696506	466.660649	466.660649	455.201362	455.201362	443.318880	443.318880	431.013355
431.013355	418.284860	418.284860	405.133410	405.133410	391.558969	391.558969	377.561457	377.561457	363.140756
363.140756	348.296715	348.296715	333.029157	333.029157	317.337879	317.337879			
J= 39									
672.858585	672.858585	666.547234	666.547234	660.512802	660.512802	654.768407	654.768406	649.331284	649.331251
644.225294	644.224712	639.488046	639.480570	635.201430	635.131835	631.593276	631.160337	628.902820	627.390210
626.469162	623.492430	623.294596	619.187748	619.160265	614.374097	614.371261	609.054491	609.054259	603.251855
603.251839	596.984150	596.984149	590.263456	590.263456	583.097997	583.097997	575.493550	575.493550	567.454288
567.454289	558.983280	558.983280	550.082818	550.082818	540.754634	540.754634	531.000037	531.000037	520.820024
520.820024	510.215346	510.215346	499.186566	499.186566	487.734097	487.734097	475.858230	475.858230	463.559157
463.559157	450.836994	450.836994	437.691784	437.691784	424.123518	424.123518	410.132139	410.132139	395.717548
395.717548	380.979611	380.879611	365.618165	365.618165	349.933019	349.933019	333.823960	333.823960	
J= 40									
707.392870	707.392870	700.912751	700.912751	694.709370	694.709370	688.795313	688.795312	683.186962	683.186944
677.906625	677.906302	672.987950	672.983555	668.497598	668.454024	664.619770	664.320553	661.660713	660.452127
659.237243	656.541147	656.231576	652.274114	652.226441	647.505893	647.500572	642.224006	642.223539	636.451113
636.451080	630.207357	630.207355	623.506490	623.506490	616.357840	616.357840	608.767932	608.767932	600.741465
600.741465	592.281890	592.281890	583.391788	583.391788	574.073106	574.073106	564.327326	564.327326	554.155577
554.155577	543.558719	543.558719	532.537401	532.537401	521.092106	521.092106	509.223183	509.223183	496.930875
496.930875	484.215336	484.215336	471.076644	471.076644	457.514820	457.514820	443.529829	443.529829	429.121594
429.121594	414.290000	414.290000	399.034899	399.034899	383.356112	383.356112	367.253438	367.253438	350.726652
350.726652									

J= 41

742.787191	742.787191	736.138146	736.138146	729.765692	729.765692	723.681923	723.681923	717.902443	717.902433
712.443206	712.448026	707.349749	707.347192	702.662629	702.635759	698.532663	698.331546	695.277442	694.345177
692.768951	690.402104	689.934226	686.165989	686.085367	681.444929	681.435171	676.204060	676.203141	670.463638
670.463568	664.245911	664.245907	657.566495	657.566495	650.435964	650.435964	642.861679	642.861679	634.848921
634.848921	626.401565	626.401565	617.522504	617.522504	608.213927	608.213927	598.477499	598.477499	588.314497
588.314497	577.725897	577.725897	566.712441	566.712441	555.274690	555.274690	543.413057	543.413057	531.127837
531.127837	518.419225	518.419225	505.287340	505.287340	491.732231	491.732231	477.753892	477.753892	463.352268
384.990345	368.045890	368.045890	433.278742	433.278742	417.606547	417.606547	401.510486	401.510486	384.990345

J= 42

779.041140	779.041140	772.223005	772.223005	765.681348	765.681348	759.427803	759.427803	753.477262	753.477257
747.344432	747.448382	742.572466	742.571012	737.693695	737.677350	733.328103	733.196134	729.767974	729.074137
727.100258	725.378170	724.397030	720.863221	720.730233	716.189554	716.172061	710.992997	710.991229	705.287988
705.287344	698.006544	693.396534	692.442327	692.442326	685.331315	685.331315	677.773804	677.773804	669.775724
669.775724	661.341415	661.341415	652.474116	652.474116	643.176276	643.176276	633.449764	633.449764	623.296014
623.296014	612.716129	612.716129	601.710955	601.710955	590.281134	590.281134	578.427149	578.427149	566.149350
566.149350	553.447982	553.447982	540.323201	540.323201	526.775092	526.775092	512.803675	512.803675	498.408922
498.408922	483.550756	483.599736	468.349064	468.349064	452.683698	452.683698	436.594482	436.594482	420.081214
420.081214	403.143670	403.143670	385.781603	385.781603					

J= 43

816.154299	816.154299	809.166905	809.166905	802.455907	802.455907	796.032509	796.032508	789.910947	789.910944
784.109910	784.109856	778.655336	778.654493	773.588595	773.578772	769.001200	768.916306	765.142489	764.643631
762.249729	760.573007	759.919450	756.365528	756.152860	751.738242	751.707587	746.589096	746.585767	740.922648
740.922348	734.763928	734.763927	728.132792	728.132792	721.042798	721.042798	713.503288	713.503288	705.520913
705.520913	697.100529	697.100528	688.245749	688.245749	678.959311	678.959311	669.243304	669.243304	659.099336
659.099336	648.528645	648.523645	637.532189	637.532189	626.110700	626.110700	614.264735	614.264735	601.994704
601.994704	589.300905	589.300905	576.183538	576.183538	562.642720	562.642720	548.678507	548.678507	534.290893
534.290893	519.479326	519.479326	504.245212	504.245212	488.586920	488.586920	472.504788	472.504788	455.998626
455.998626	439.068221	439.068221	421.713337	421.713337	403.933721	403.933721			

J= 44

854.126238	854.126238	846.969410	846.969410	840.088926	840.088926	833.495586	833.495586	827.203022	827.203020
821.228957	821.228927	815.597559	815.597081	810.345604	810.339766	805.547216	805.493563	801.405400	801.057891
798.236946	796.861181	795.607317	792.674642	792.344225	788.089699	788.037200	782.990596	782.984458	777.366027
777.365457	771.246676	771.240633	764.636654	764.636651	757.569280	757.569280	750.049077	750.049077	742.083495
742.083495	733.677958	733.677958	724.836499	724.836499	715.562163	715.562163	705.857280	705.857280	695.723646
695.723646	685.162650	685.162650	674.175368	674.175368	662.762630	662.762630	650.925071	650.925071	638.663170
638.663170	625.977278	625.977278	612.867642	612.867642	599.334419	599.334419	585.377697	585.377697	570.997500
570.997500	556.193798	556.193798	540.966519	540.966519	525.315551	525.315551	509.240746	509.240746	492.741930
492.741930	475.818898	475.818898	458.471427	458.471427	440.699271	440.699271	422.502166	422.502166	

J= 45

892.956517	892.956517	885.630077	885.630077	878.579954	878.579954	871.816571	871.816571	865.353001	865.353000
859.206089	859.206073	853.398472	853.398204	847.963344	847.959910	842.962396	842.928702	838.556018	838.320571
835.080814	834.037234	832.372596	829.792385	829.295726	825.243002	825.155193	820.195724	820.184643	814.616458
814.615358	808.527334	808.527244	801.952617	801.952611	794.909583	794.909583	787.410078	787.410078	779.462446
779.462446	771.072735	771.072735	762.245436	762.245436	752.983937	752.983937	743.290828	743.290828	733.168109
733.168109	722.617330	722.617330	711.639696	711.639696	700.236143	700.236143	688.407394	688.407394	676.153996
676.153996	663.476362	663.476362	650.374787	650.374787	636.849471	636.849471	622.900538	622.900538	608.528041
608.528041	593.731978	593.731978	578.512300	578.512300	562.868911	562.868911	546.801684	546.801684	530.310456
530.310456	513.395037	513.395037	496.055214	496.055214	478.290749	478.290749	460.101390	460.101390	441.486863
441.486863									

TABLE III—*Continued*

J= 46									
932.644684	932.644684	925.148447	925.148447	917.928526	917.928526	910.994991	910.994991	904.360391	904.360391
898.040774	898.040765	892.057428	892.057275	886.440678	886.438678	881.242576	881.222073	876.590394	876.434628
872.757454	872.016162	869.931917	867.721687	867.001376	863.197754	863.054474	858.202755	858.183165	852.672199
852.670120	846.622375	846.622195	840.079334	840.079321	833.062486	833.062485	825.585163	825.585163	817.656705
817.655755	809.283855	809.283855	800.471603	800.471603	791.223713	791.223713	781.543059	781.543059	771.431861
771.431861	760.851844	760.851844	749.924355	749.924355	738.530441	738.530441	726.710918	726.710918	714.466413
714.466413	701.797398	701.797398	688.704225	688.704225	675.187139	675.187139	661.246301	661.246301	646.881798
646.881798	632.093656	632.093656	616.881849	616.881849	601.246304	601.246304	585.186909	585.186909	568.703518
568.703518	551.795956	551.795956	534.464020	534.464020	516.707484	516.707484	498.526102	498.526102	479.919610
479.919610	460.887727	460.887727							
J= 47									
973.190275	973.190275	965.524052	965.524052	958.134169	958.134169	951.030361	951.030361	944.224691	944.224691
937.733474	937.732469	931.573830	931.573717	925.775633	925.775478	920.386594	920.373659	915.503263	915.402289
911.398073	910.832748	908.304785	906.466309	905.460236	901.054245	901.726553	897.010094	896.976186	891.531445
891.527593	885.524201	885.523847	879.015396	879.015369	872.026720	872.026718	864.573163	864.573163	856.665179
856.665179	848.310283	848.310283	839.514014	839.514014	830.280545	830.280545	820.613058	820.613058	810.514016
810.514016	799.965332	799.965332	789.028504	789.028504	777.644701	777.644701	765.834839	765.834839	753.599628
753.599628	740.939609	740.939609	727.855191	727.855191	714.346667	714.346667	700.414241	700.414241	686.058033
686.058033	671.278102	671.278102	656.074444	656.074444	640.447012	640.447012	624.395711	624.395711	607.920414
607.922414	591.020958	591.020958	573.697154	573.697154	556.048736	555.948786	537.775619	537.775619	519.177396
519.177396	500.153844	500.153844	480.704675	480.704675					
J= 48									
1014.592316	1014.592316	1006.756412	1006.756412	999.196396	999.196396	991.922185	991.922185	984.945390	984.945390
978.280648	978.280645	971.946975	971.946929	965.970345	965.969684	960.390636	960.383178	955.289396	955.225079
950.697322	950.491407	947.511888	946.330686	944.677985	941.513588	941.162020	936.616388	936.558939	931.192348
931.185350	925.231133	925.230448	918.759334	918.759278	911.800964	911.800960	904.372865	904.372865	896.486740
896.486740	888.150953	883.150953	879.371653	879.371653	870.153457	870.153457	860.499888	860.499888	850.413666
850.413666	839.896910	839.896910	828.951280	828.951280	817.578079	817.578079	805.778330	805.778330	793.552830
793.552830	780.902196	780.902196	767.826897	767.826897	754.327281	754.327281	740.403592	740.403592	726.055991
726.055991	711.284566	711.284566	696.089345	696.089345	680.470302	680.470302	664.427364	664.427364	647.960420
647.960420	631.069325	631.069325	613.753902	613.753902	596.013949	596.013949	577.849238	577.849238	559.259522
559.259522	540.244537	540.244537	520.804000	520.804000	500.937617	500.937617			
J= 49									
1056.851820	1056.851820	1048.845037	1048.845037	1041.114710	1041.114710	1033.669957	1033.669957	1026.521966	1026.521966
1019.684747	1019.684746	1013.176344	1013.176319	1007.021022	1007.020646	1001.254591	1001.250165	995.944244	995.903899
991.266343	990.905965	987.573294	986.419700	984.666824	981.877807	981.351847	977.020660	976.925465	971.653056
971.642589	965.741414	965.740116	959.309607	959.309495	952.383845	952.383837	944.983017	944.983016	937.120219
937.120219	928.804766	928.804766	920.043474	920.043474	910.841449	910.841449	901.202581	901.202581	891.129874
891.129874	880.625668	880.625668	869.691798	869.691798	858.329710	858.329710	846.540542	846.540542	834.325187
834.325187	821.684341	821.684341	808.618539	808.618539	795.128184	795.128184	781.213569	781.213569	766.874894
766.874894	752.112283	752.112283	736.925793	736.925793	721.315421	721.315421	705.281120	705.281120	688.822798
688.822798	671.940324	671.940324	654.633537	654.633537	636.902247	636.902247	618.746238	618.746238	600.165273
600.165273	581.159094	581.159094	561.727428	561.727428	541.869984	541.869984	521.586462	521.586462	
J= 50									
1099.966790	1099.966790	1091.789424	1091.789424	1083.888602	1083.888602	1076.273161	1076.273161	1068.953889	1068.953889
1061.944218	1061.944217	1055.261303	1055.261290	1048.927917	1048.927705	1042.976636	1042.974034	1037.464103	1037.439139
1032.529610	1032.246542	1028.606261	1027.638407	1025.444035	1023.049860	1022.289599	1018.222472	1018.068375	1012.911765
1012.389984	1007.653213	1007.650793	1000.664602	1000.664382	993.773932	993.773915	986.402316	986.402315	978.564411
978.564411	970.270587	970.270587	961.528399	961.528399	952.343489	952.343489	942.720146	942.720146	932.661681
932.661681	922.170673	922.170673	911.249149	911.249149	899.898706	899.898706	888.120606	888.120606	875.915845
875.915845	863.285204	863.285204	850.229289	850.229289	836.748562	836.748562	822.843368	822.843368	808.513949
808.513949	793.760466	793.760466	778.583007	778.583007	762.981600	762.981600	746.956217	746.956217	730.506788
730.506788	713.633201	713.633201	696.335311	696.335311	678.612939	678.612939	660.465883	660.465883	641.893916
641.893916	622.896787	622.896787	603.474232	603.474232	583.625967	583.625967	563.351697	563.351697	542.651112
542.651112									

H_K as a variable. The spectral constants have been used to generate the energy levels shown in Table III. Because of the large number of rotational lines, the calculated spectrum is not reproduced here. It is available either from the Editorial Office of this Journal or from the second author.

An important point should be made about the use of these data in conjunction with other data sets, especially infrared rotation–vibration data sets. Although accurate ground-state energy levels are a convenient starting point for spectra assignments, from a statistical point of view it is preferable to use the observed microwave data directly in the final spectral analysis. The appropriate weightings for data are then reasonably straightforward. On the other hand, if energy levels or spectral constants are used, the appropriate statistical treatment requires the consideration of both the uncertainties in the spectral constants and in the correlation matrix (*18*). This is especially important in large centrifugal distortion analyses because of the significant correlations among the constants.

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