JOURNAL OF MOLECULAR SPECTROSCOPY **114**, 377–394 (1985)

The $\nu_1 + \nu_2$ and $\nu_1 + \nu_2 - \nu_2$ Bands of $^{14}NH_3$ and $^{15}NH_3$

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The $\nu_1 + \nu_2$ and $\nu_1 + \nu_2 - \nu_2$ bands of $^{14}NH_3$ and $^{15}NH_3$ have been assigned in the Fourier transform spectra measured with a resolution of 0.02 cm^{-1}. The effective molecular parameters describing inversion–rotation energy levels of the $\nu_1 + \nu_2$ vibrational state have been obtained, including off-diagonal $\Delta k = \pm 3$ vibration–rotation interactions. In the case of $^{15}NH_3$, the analysis of these bands has been performed for the first time. © 1985 Academic Press, Inc.

I. INTRODUCTION

The first measurement of the $\nu_1 + \nu_2$ band with resolution sufficient to resolve the entire rotational structure was carried out by Benedict *et al.* (*1*), who also presented a basic analysis including a determination of the molecular parameters of the $\nu_1 + \nu_2$ state. More recently, Margolis and Kwan (*2*) have measured the absorption strengths of some $\nu_1 + \nu_2$ transitions and obtained the intensity parameters for this band.

In the present paper we report a frequency analysis of the $\nu_1 + \nu_2$ band of $^{14}NH_3$, using Fourier transform spectra with wavenumber precision and spectral resolution nearly two orders of magnitude better than in the previous studies (*1, 2*). In addition, we present also a frequency analysis of the $\nu_1 + \nu_2 - \nu_2$ "hot" band. Both bands were analyzed simultaneously, and thereby a single set of spectroscopic parameters describing the $\nu_1 + \nu_2$ energy levels was derived. Along with this analysis an analogous study of the $\nu_1 + \nu_2$ and $\nu_1 + \nu_2 - \nu_2$ bands was also carried out for the isotopic species $^{15}NH_3$. In this case, the analysis has been done for the first time.

II. EXPERIMENT AND LINE ASSIGNMENTS

The Fourier transform spectra were obtained by means of a 1-m Fourier interferometer at the Kitt Peak National Observatory in Tucson, Arizona. The measurements were carried out with a single cell 150 cm long at a sample pressure of 0.5 Torr for $^{14}NH_3$ and 1.0 Torr for $^{15}NH_3$. Besides, measurements with a 6-m multipass White-type absorption cell using an optical pathlength of 96 m were made at gas pressures of 0.75 and 3.0 Torr for $^{14}NH_3$ and at pressures of 0.1 and 2.0 Torr for $^{15}NH_3$ (see Figs. 1 and 2). The spectra were calibrated against the difference frequency laser measurements of the ν_1 band of $^{14}NH_3$ as indicated in Ref. (*3*), and from this calibration the absolute accuracy of the wavenumbers of isolated lines is estimated to be about 0.002 cm^{-1}.

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0022-2852/85 $3.00
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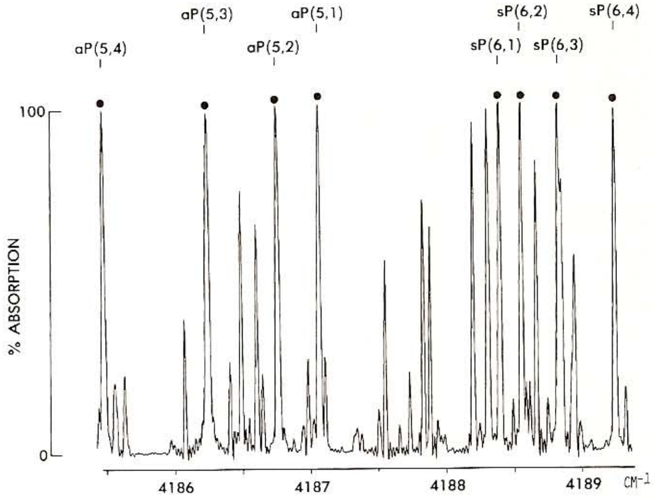

FIG. 1. Part of the Fourier transform spectra recorded at 2 Torr of $^{15}NH_3$, using a path length of 96 m, with several assigned $\nu_1 + \nu_2$ band transitions.

The assignments of the $\nu_1 + \nu_2$ band transitions in $^{14}NH_3$ have been performed following the previous analysis (*1*). The identification of the $\nu_1 + \nu_2 - \nu_2$ hot band transitions was carried out simultaneously with the analysis of the $\nu_1 + \nu_2$ band, using the values of the ground state and the ν_2-state energy levels derived in Ref. (*4*). In this

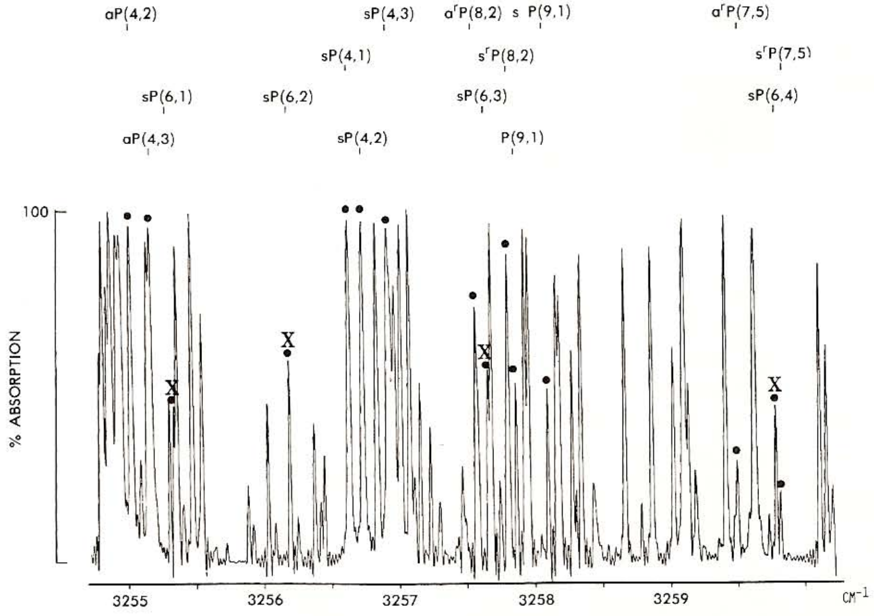

FIG. 2. Part of the Fourier transform spectra recorded at 2 Torr of $^{15}NH_3$, using a pathlength of 96 m. Full dots with X over them ($\overset{X}{\bullet}$) indicate lines corresponding to the $\nu_1 + \nu_2 - \nu_2$ band transitions, while full dots (●) refer to the ν_1 and ν_3 band transitions.

way, a set of additional control differences between wavenumbers of the $\nu_1 + \nu_2$ and $\nu_1 + \nu_2 - \nu_2$ band transitions was obtained. These extra differences were found to be very useful, especially in cases where the usual combination differences were inapplicable or missing due to overlaps of lines or because of selection rules (for $J = K$, $J = K + 1$, and $K = 0$). To assist the identification procedure, intensities of assigned transitions were also calculated. The calculations were performed neglecting all the rotation–vibration interactions, using the Margolis and Kwan $\nu_1 + \nu_2$ transition moment (*2*), and assuming the $\nu_1 + \nu_2 - \nu_2$ transition moment to be the same as the ν_1 transition moment of Ref. (*5*).

In the case of $^{15}NH_3$, the procedure of analysis was different as no study pertaining to the $\nu_1 + \nu_2$ states of this isotopic species has been performed so far. The analysis was based on the knowledge of precise values of the ground and ν_2 state energy levels given in Ref. (*6*). A simple computer program was written to search for a sextet of transitions to the same upper energy level (three $\nu_1 + \nu_2$ band and three $\nu_1 + \nu_2 - \nu_2$ band transitions) that simultaneously satisfied all the combination differences between the energy levels in the ground and ν_2 states. The wavenumber interval for the search of these transitions was estimated using the values of vibrational energies calculated from the potential function (*7*). After assigning a sufficient number of transitions, which allowed the determination of the band origin and the rotational constants of the $\nu_1 + \nu_2$ state, the continuation of the analysis was performed in the same manner as for $^{14}NH_3$, using the same values of the transition moments in the intensity calculations.

III. THE $\nu_1 + \nu_2$ VIBRATIONAL STATE

The nondegenerate $\nu_1 + \nu_2$ vibrational state belongs to a complex interacting system involving the degenerate $\nu_3 + \nu_2$, $2\nu_4 + \nu_2(E)$, $3\nu_2 + \nu_4$, and the nondegenerate $2\nu_4 + \nu_2(A)$, $4\nu_2$, $5\nu_2$ vibrational states (see Fig. 3). In this system the essential vibration–

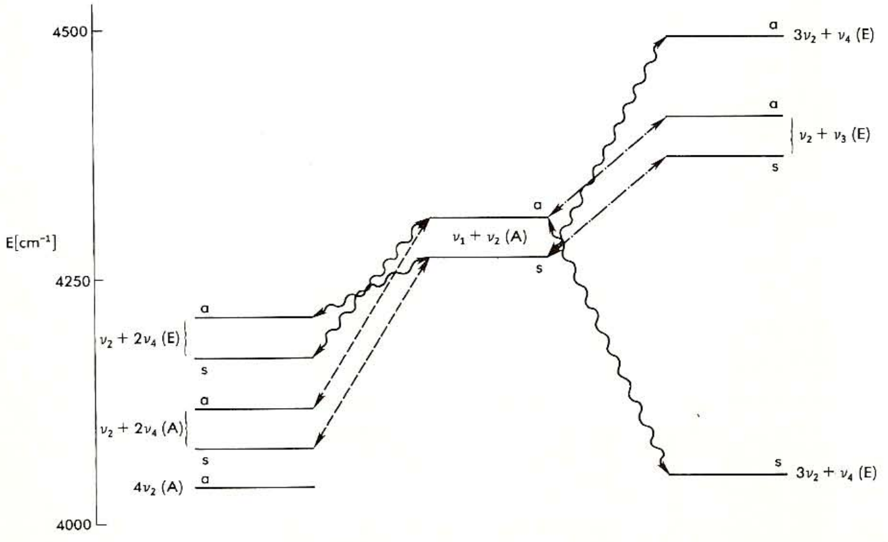

FIG. 3. The essential vibration–rotation interactions of the $\nu_1 + \nu_2$ state. Wavy lines refer to the Coriolis interactions, dash–dot lines to the *K*-type interactions, and the dashed lines to the Fermi interactions.

rotation perturbations of the $\nu_1 + \nu_2$ state are expected to be analogous to those discussed in connection with the ν_1 vibrational state (*1, 3*). Therefore, due to an interlevel crossing of the corresponding energy levels, a higher-order *x*, *y*–Coriolis interaction between the $|v_1 = 1, v_2 = 1^{\mp}, v_3 = 0^0, v_4 = 0^0; J, K\rangle$ and $|v_1 = 0, v_2 = 1^{\pm}, v_3 = 0^0, v_4 = 2^{\mp 2}; J, K \pm 1\rangle$ states would cause the crucial perturbations. The *x*, *y*–Coriolis interaction between the $\nu_1 + \nu_2(A)$ and $\nu_2 + \nu_3(E)$ vibrational states is much less significant because of a negligible value for the $\zeta^x_{1,3}$ Coriolis constant (*8*). Stronger perturbations of the $\nu_1 + \nu_2$ state can be expected, however, due to the *K*-type interactions ($\nu_2 + \nu_3$ state) and the Fermi interactions [$2\nu_4 + \nu_2(A)$ state]. In addition, there are also significant *x*, *y*–Coriolis interactions between the $\nu_1 + \nu_2$ and $\nu_1 + \nu_4$, $\nu_1 + 2\nu_2$, etc., states which are similar to the strong perturbations between the ν_2 and ν_4, $2\nu_2$, etc., states (*9, 10*). The similarity of the $\nu_1 + \nu_2$ state to the ν_2 vibrational state is also indicated by the inversion splitting of about 25 cm^{-1}, which is comparable to the rotational spacing, and thus the effect of the $\Delta k = 3$ interaction (*4*) might be significant.

It is obvious that a detailed analysis of the $\nu_1 + \nu_2$ state represents a formidable numerical task that requires the simultaneous treatment of many vibrational bands. Such an approach is complicated by the fact that the assignments of all of these bands [except the $\nu_2 + \nu_3$ band of $^{14}\text{NH}_3$ (*1*)] have not been performed so far and would be very difficult because of the weak intensities of some of these bands. On the other hand, for low values of the rotational quantum numbers, the off-diagonal rotation–vibration interactions do not have the resonance character; therefore, in this case the perturbation effect can be absorbed into the centrifugal distortion constants of higher order (*11*). Thus, in the first attempt, the following expansion is used for a description of the $\nu_1 + \nu_2$ state energy levels:

$$\begin{aligned} {}^{(i)}E(J, K) = {} & {}^{(i)}E_0 + {}^{(i)}BJ(J+1) + ({}^{(i)}C - {}^{(i)}B)K^2 - {}^{(i)}D_J J^2(J+1)^2 \\ & - {}^{(i)}D_{JK}J(J+1)K^2 - {}^{(i)}D_K K^4 + {}^{(i)}H_{JJJ}J^3(J+1)^3 \\ & + {}^{(i)}H_{JJK}J^2(J+1)^2K^2 + {}^{(i)}H_{JKK}J(J+1)K^4 + {}^{(i)}H_{KKK}K^6 \\ & + {}^{(i)}G_{JJJJ}J^4(J+1)^4 + {}^{(i)}\mathrm{G}_{JJJK}\mathrm{J}^3(J+1)^3K^2 + {}^{(i)}G_{JJKK}J^2(J+1)^2K^4 \\ & \qquad + {}^{(i)}G_{JKKK}J(J+1)K^6 + {}^{(i)}G_{KKKK}K^8 \pm \eta_3(-1)^J[(J+3)!/(J-3)!]\delta_{K,3}, \end{aligned}$$

where all the parameters are expressed in units of cm^{-1}; *i* indicates the inversion parity *s* or *a*, and η_3 is a correction from the off-diagonal matrix element with $\Delta k = \pm 6$ that contributes for the special case $K = 3$ ($K = |k|$) to the diagonal. The upper and lower signs before the last term refer to the *s* and *a* inversion components, respectively; and $\delta_{K,3}$ is the Kronecker symbol. In addition to this, the $\Delta k = \pm 3$ off-diagonal matrix elements (*4*),

$$\langle \binom{s}{a}; J, k | \alpha[(J_+^3 + J_-^3)J_z + J_z(J_+^3 + J_-^3)] | \binom{a}{s}; J, k \pm 3 \rangle,$$

were included in the parametrization scheme, since one can expect these off-diagonal matrix elements to be determinable in a manner similar to those for the ν_2 state (*4, 6*).

IV. RESULTS AND CONCLUSIONS

Wavenumbers of all the assigned transitions are collected in Tables I–IV. All these transitions to the $\nu_1 + \nu_2$ state have been processed in a least-squares analysis with

TABLE I

Transition Wavenumbers (cm^{-1}) and Intensities (cm^{-2} atm^{-1}) of the $\nu_1 + \nu_2$ Band of $^{14}NH_3$

			sP(J,K)						aP(J,K)		
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
1	0	4300.1399	4300.1434(100)	35	0.17E-1	1	0	(4273.8360)	-------	----	0.0
2	0	(4279.8755)	-------	----	0.0	2	0	4253.8480	4253.8505(50)	25	0.29E-1
2	1	4279.9575	4279.9598(20)	23	0.11E-1	2	1	4253.7455	4253.7450(50)	-5	0.11E-1
3	0	4259.2647	4259.2645(20)	-1	0.31E-1	3	0	(4233.7696)	-------	----	0.0
3	1	4259.3411	4259.3426(50)	16	0.14E-1	3	1	4233.6661	4233.6630(500)	-30	0.15E-1
3	2	4259.5740	4259.5692(30)	-47	0.93E-2	3	2	4233.3507	4233.3466(50)	-40	0.97E-2
4	0	(4238.3428)	-------	----	0.0	4	0	4213.6168	4213.6161(500)	-6	0.29E-1
4	1	4238.4121	4238.4091(30)	-30	0.13E-1	4	1	4213.5128	4213.5146(20)	18	0.14E-1
4	2	4238.6244	4238.6239(50)	-4	0.11E-1	4	2	4213.1962	4213.1981(50)	19	0.12E-1
4	3	4238.9917	4238.9872(50)	-44	0.14E-1	4	3	4212.6538	4212.6552(50)	13	0.15E-1
5	0	4217.1516	4217.1513(20)	-3	0.21E-1	5	0	(4193.4047)	-------	----	0.0
5	1	4217.2126	4217.2099(50)	-26	0.10E-1	5	1	4193.3004	4193.2997(30)	-5	0.11E-1
5	2	4217.3999	4217.4013(30)	14	0.97E-2	5	2	4192.9835	4192.9794(30)	-40	0.10E-1
5	3	4217.7265	4217.7294(50)	29	0.16E-1	5	3	4192.4425	4192.4443(30)	18	0.17E-1
5	4	4218.2130	4218.2177(500)	47	0.52E-2	5	4	4191.6560	4191.6513(50)	-46	0.54E-2
6	0	(4195.7410)	-------	----	0.0	6	0	4173.1495	4173.1513(50)	19	0.15E-1
6	1	4195.7918	4195.7958(100)	40	0.71E-2	6	1	4173.0446	4173.0380(50)	-64	0.74E-2
6	2	4195.9490	4195.9482(500)	-8	0.68E-2	6	2	4172.7271	4172.7255(30)	-14	0.71E-2
6	3	4196.2274	4196.2255(50)	-17	0.13E-1	6	3	4172.1863	4172.1826(30)	-36	0.13E-1
6	4	4196.6480	4196.6513(50)	33	0.53E-2	6	4	4171.4070	4171.4091(50)	22	0.55E-2
6	5	4197.2402	4197.2411(30)	9	0.34E-2	6	5	4170.3567	4170.3544(50)	-21	0.36E-2
7	0	4174.1722	4174.1787(500)	64	0.84E-2	7	0	(4152.8720)	-------	----	0.0
7	1	4174.2110	4174.2138(50)	29	0.42E-2	7	1	4152.7659	4152.7607(500)	-51	0.44E-2
7	2	4174.3320	4174.3310(30)	-9	0.42E-2	7	2	4152.4461	4152.4443(30)	-17	0.43E-2
7	3	4174.5485	4174.5459(100)	-26	0.81E-2	7	3	4151.9072	4151.9092(50)	19	0.84E-2
7	4	4174.8913	4174.8974(500)	61	0.38E-2	7	4	4151.1307	4151.1279(50)	-27	0.39E-2
7	5	4175.3886	4175.3857(50)	-28	0.32E-2	7	5	4150.0982	4150.0928(100)	-53	0.34E-2
7	6	4176.0757	4176.0771(50)	14	0.43E-2	7	6	4148.7574	4148.7529(50)	-44	0.45E-2
8	0	(4152.5287)	-------	----	0.0	8	0	4132.6034	4132.6006(20)	-27	0.46E-2
8	1	4152.5529	4152.5537(30)	8	0.22E-2	8	1	4132.4950	4132.4951(30)	1	0.23E-2
8	2	4152.6303	4152.6318(20)	15	0.22E-2	8	2	4132.1707	4132.1709(30)	2	0.23E-2
8	3	4152.7796	4152.7842(500)	45	0.45E-2	8	3	4131.6217	4131.6201(30)	-15	0.47E-2
8	4	4153.0174	4153.0185(50)	12	0.22E-2	8	4	4130.8547	4130.8506(100)	-40	0.23E-2
8	5	4153.3936	4153.3935(30)	0	0.21E-2	8	5	4129.8407	4129.8350(100)	-56	0.22E-2
8	6	4153.9496	4153.9443(50)	-51	0.37E-2	8	6	4128.5443	4128.3154(50)[a]	-2287	0.38E-2
8	7	4154.7217	4154.7217(30)	0	0.12E-2	8	7	4126.8694	4126.8936(100)[a]	242	0.13E-2
9	0	4130.9337	-------	----	0.21E-2	9	0	(4112.3941)	-------	----	0.0
9	1	4130.9402	4130.9404(50)	2	0.10E-2	9	1	4112.2821	4112.2803(30)	-17	0.11E-2
9	2	4130.9647	4130.9639(100)	-8	0.11E-2	9	2	4111.9505	4111.9522(30)	16	0.11E-2
9	3	4131.0120	4131.0225(100)[a]	105	0.22E-2	9	3	4111.4083	4111.4092(30)	9	0.23E-2
9	4	4131.1378	4131.1436(30)[a]	58	0.11E-2	9	4	4110.6289	4110.6592(30)[a]	303	0.12E-2
9	5	4131.3585	4131.3584(30)	0	0.11E-2	9	5	4109.6356	4109.6358(30)	2	0.12E-2
9	6	4131.7385	4131.7334(100)	-50	0.22E-2	9	6	4108.3928	4108.3389(100)[a]	-538	0.23E-2
9	7	4132.3351	4132.3350(30)	-1	0.98E-3	9	7	4106.8207	4106.7647(100)[a]	-559	0.10E-2
9	8	4133.1803	4133.1787(30)	-15	0.68E-3	9	8	4104.7269	4104.7256(50)	-12	0.71E-3
10	0	(4109.5812)	-------	----	0.0	10	0	4092.3260	4092.3226(30)[a]	-33	0.92E-3
10	1	4109.5663	4109.5694(50)	31	0.44E-3	10	1	4092.2093	4092.2095(20)	3	0.46E-3
10	2	4109.5263	4109.5225(30)	-37	0.45E-3	10	2	4091.8689	4091.8702(20)	12	0.47E-3
10	3	4109.4872	4109.4678(100)[a]	-193	0.94E-3	10	3	4091.2910	4091.2510(50)[a]	-398	0.98E-3
10	4	4109.4318	4109.4287(50)	-30	0.49E-3	10	4	4090.5411	4090.4175(50)[a]	-1234	0.51E-3
10	5	4109.4520	4109.4561(30)	41	0.51E-3	10	5	4089.5750	4089.2923(30)[a]	-2826	0.53E-3
10	6	4109.5961	4109.5928(30)	-32	0.11E-2	10	6	4088.4021	-------	----	0.11E-2
10	7	4109.9413	4109.8780(30)[a]	-632	0.53E-3	10	7	4086.9637	4086.7442(50)[a]	-2194	0.56E-3
10	8	4110.5555	4110.5889(30)[a]	334	0.49E-3	10	8	4085.0914	4084.1602(50)[a]	-9311	0.51E-3
10	9	4111.4542	-------	----	0.71E-3	10	9	4082.4097	4082.5587(500)[a]	1489	0.73E-3
11	0	4088.7833	4088.8516(100)[a]	683	0.34E-3						
11	1	4088.7421	4088.3873(500)[a]	-3548	0.17E-3						
11	2	4088.6229	-------	----	0.17E-3						
11	3	4088.3990	4088.4944(500)[a]	954	0.36E-3						
11	4	4088.1924	-------	----	0.19E-3						
11	5	4087.9541	-------	----	0.21E-3						
11	6	4087.7841	4087.8753(30)[a]	912	0.44E-3						
11	7	4087.7767	4087.6907(30)[a]	-859	0.24E-3						
11	8	4088.0344	4088.1551(100)[a]	1207	0.24E-3						
11	9	4088.6314	4088.5184(100)[a]	-1130	0.46E-3						
11	10	4089.5464	4089.5601(100)[a]	137	0.17E-3						

[a] Lines not used in the least squares fit in obtaining molecular parameters.

TABLE I—*Continued*

sQ(J,K)						aQ(J,K)					
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
0	0	(4320.0298)	-------	----	0.0	0	0	(4293.7158)	-------	----	0.0
1	0	(4319.6349)	-------	----	0.0	1	0	(4293.5877)	-------	----	0.0
1	1	4319.7232	4319.7215(30)	-16	0.13E-1	1	1	4293.4914	4293.4910(30)	-3	0.14E-1
2	0	(4318.8532)	-------	----	0.0	2	0	(4293.3295)	-------	----	0.0
2	1	4318.9389	4318.9363(30)	-25	0.60E-2	2	1	4293.2351	4293.2371(20)	20	0.63E-2
2	2	4319.2001	4319.1980(20)	-19	0.25E-1	2	2	4292.9471	4292.9442(500)	-29	0.26E-1
3	0	(4317.7001)	-------	----	0.0	3	0	(4292.9378)	-------	----	0.0
3	1	4317.7819	4317.7801(30)	-17	0.31E-2	3	1	4292.8458	4292.8426(50)	-31	0.33E-2
3	2	4318.0314	4318.0301(30)	-13	0.13E-1	3	2	4292.5655	4292.5652(30)	-1	0.14E-1
3	3	4318.4612	4318.4597(30)	-14	0.65E-1	3	3	4292.0839	4292.0887(50)	48	0.68E-1
4	0	(4316.1983)	-------	----	0.0	4	0	(4292.4085)	-------	----	0.0
4	1	4316.2745	4316.2761(500)	16	0.16E-2	4	1	4292.3191	4292.3192(30)	1	0.17E-2
4	2	4316.5080	4316.5066(50)	-12	0.69E-2	4	2	4292.0472	4292.0457(50)	-13	0.72E-2
4	3	4316.9120	4316.9051(500)	-68	0.34E-1	4	3	4291.5812	4291.5809(30)	-3	0.35E-1
4	4	4317.5075	4317.5066(30)	-8	0.34E-1	4	4	4290.9010	4290.8973(50)	-37	0.36E-1
5	0	(4314.3788)	-------	----	0.0	5	0	(4291.7395)	-------	----	0.0
5	1	4314.4478	4314.4480(30)	2	0.82E-3	5	1	4291.6524	4291.6512(50)	-11	0.85E-3
5	2	4314.6597	4314.6629(100)	32	0.35E-2	5	2	4291.3882	4291.3856(30)	-25	0.36E-2
5	3	4315.0292	4315.0262(50)	-29	0.17E-1	5	3	4290.9372	4290.9363(500)	-7	0.18E-1
5	4	4315.5795	4315.5730(500)	-64	0.17E-1	5	4	4290.2832	4290.2840(30)	8	0.18E-1
5	5	4316.3400	4316.3387(20)	-13	0.32E-1	5	5	4289.3964	4289.3973(30)	8	0.33E-1
6	0	(4312.2857)	-------	----	0.0	6	0	(4290.9341)	-------	----	0.0
6	1	4312.3452	-------	----	0.39E-3	6	1	4290.8484	4290.8504(100)	20	0.40E-3
6	2	4312.5291	4312.5262(50)	-29	0.16E-2	6	2	4290.5901	4290.5848(50)	-52	0.17E-2
6	3	4312.8520	4312.8543(100)	23	0.80E-2	6	3	4290.1527	4290.1512(30)	-14	0.84E-2
6	4	4313.3422	4313.3426(100)	4	0.81E-2	6	4	4289.5224	4289.5223(30)	0	0.84E-2
6	5	4314.0327	4314.0340(50)	13	0.15E-1	6	5	4288.6780	4288.6746(100)	-32	0.16E-1
6	6	4314.9595	4314.9597(30)	3	0.52E-1	6	6	4287.5701	4287.5692(20)	-8	0.55E-1
7	0	(4309.9851)	-------	----	0.0	7	0	(4290.0067)	-------	----	0.0
7	1	4310.0327	4310.0301(50)	-26	0.17E-3	7	1	4289.9213	-------	----	0.18E-3
7	2	4310.1807	4310.1824(30)	17	0.72E-3	7	2	4289.6660	4289.6707(30)	47	0.75E-3
7	3	4310.4456	4310.4441(30)	-13	0.35E-2	7	3	4289.2355	4289.2371(30)	16	0.37E-2
7	4	4310.8529	4310.8543(30)	14	0.35E-2	7	4	4288.6288	4288.6277(50)	-10	0.37E-2
7	5	4311.4461	4311.4480(30)	20	0.65E-2	7	5	4287.8266	4287.8192(100)	-73	0.68E-2
7	6	4312.2711	4312.2723(30)	12	0.23E-1	7	6	4286.7922	4286.5614(30)[a]	-2307	0.24E-1
7	7	4313.3667	4313.3660(50)	-6	0.20E-1	7	7	4285.4316	4285.4559(500)[a]	243	0.21E-1
8	0	(4307.5849)	-------	----	0.0	8	0	(4288.9917)	-------	----	0.0
8	1	4307.6173	4307.6160(100)	-12	0.69E-4	8	1	4288.9051	-------	----	0.72E-4
8	2	4307.7197	4307.7176(100)	-20	0.29E-3	8	2	4288.6500	-------	----	0.30E-3
8	3	4307.9030	4307.9129(30)[a]	99	0.14E-2	8	3	4288.2299	4288.2293(50)	-5	0.15E-2
8	4	4308.2074	4308.2098(30)	24	0.14E-2	8	4	4287.6367	4287.6629(50)[a]	262	0.15E-2
8	5	4308.6675	4308.6668(30)	-6	0.26E-2	8	5	4286.8775	4286.8778(50)	3	0.28E-2
8	6	4309.3441	4309.3426(30)	-15	0.93E-2	8	6	4285.9244	-------	----	0.97E-2
8	7	4310.2974	4310.2996(500)	22	0.80E-2	8	7	4284.6997	4284.6434(500)[a]	-562	0.83E-2
8	8	4311.5625	4311.5574(100)	-50	0.14E-1	8	8	4283.0137	4283.0145(100)	8	0.14E-1
9	0	(4305.2643)	-------	----	0.0	9	0	(4287.9564)	-------	----	0.0
9	1	4305.2776	-------	----	0.26E-4	9	1	4287.8673	-------	----	0.27E-4
9	2	4305.3223	-------	----	0.11E-3	9	2	4287.6103	-------	----	0.11E-3
9	3	4305.4148	4305.3934(30)[a]	-213	0.54E-3	9	3	4287.1825	-------	----	0.56E-3
9	4	4305.5701	4305.5652(50)	-47	0.54E-3	9	4	4286.6185	4286.4910(50)[a]	-1274	0.56E-3
9	5	4305.8506	4305.8543(20)	37	0.99E-3	9	5	4285.9077	4285.6278(500)[a]	-2798	0.10E-2
9	6	4306.3173	4306.3113(50)	-59	0.35E-2	9	6	4285.0506	4284.6707(500)[a]	-3797	0.36E-2
9	7	4307.0500	4306.9832(50)[a]	-667	0.30E-2	9	7	4283.9907	4283.7645(100)[a]	-2262	0.31E-2
9	8	4308.1204	4308.1512(100)[a]	307	0.51E-2	9	8	4282.5627	4281.6317(500)[a]	-9310	0.53E-2
9	9	4309.5482	4309.6082(20)[a]	600	0.18E-1	9	9	4280.3946	4280.5379(50)[a]	1433	0.18E-1
10	0	(4303.3219)	-------	----	0.0						
10	1	4303.3110	-------	----	0.89E-5						
10	2	4303.2829	-------	----	0.38E-4						
10	3	4303.2299	-------	----	0.19E-3						
10	4	4303.2204	-------	----	0.19E-3						
10	5	4303.2619	-------	----	0.34E-3						
10	6	4303.4385	4303.5301(30)[a]	915	0.12E-2						
10	7	4303.8474	4303.7645(30)[a]	-828	0.10E-2						
10	8	4304.5947	4304.7137(50)[a]	1190	0.17E-2						
10	9	4305.7593	4305.6434(30)[a]	-1159	0.60E-2						
10	10	4307.3255	4307.3348(100)[a]	92	0.53E-2						

TABLE I—*Continued*

		sR(J,K)						aR(J,K)			
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
0	0	(4339.5248)	-------	----	0.0	0	0	4313.4676	4313.4676(30)	0	0.20E-1
1	0	4358.6127	4358.6120(30)	-5	0.35E-1	1	0	(4333.0693)	-------	----	0.0
1	1	4358.7047	4358.7058(30)	11	0.13E-1	1	1	4332.9810	4332.9793(20)	-16	0.14E-1
2	0	(4377.2886)	-------	----	0.0	2	0	4352.4977	4352.4949(20)	-27	0.45E-1
2	1	4377.3797	4377.3816(30)	18	0.19E-1	2	1	4352.4148	4352.4128(30)	-19	0.20E-1
2	2	4377.6575	4377.6589(30)	14	0.13E-1	2	2	4352.1619	4352.1628(30)	9	0.13E-1
3	0	4395.5556	4395.5534(50)	-21	0.43E-1	3	0	(4371.7294)	-------	----	0.0
3	1	4395.6442	4395.6433(30)	-9	0.21E-1	3	1	4371.6521	4371.6550(30)	29	0.21E-1
3	2	4395.9150	4395.9167(500)	17	0.17E-1	3	2	4371.4164	4371.4128(50)	-35	0.18E-1
3	3	4396.3815	4396.3815(30)	1	0.22E-1	3	3	4371.0113	4371.0066(30)	-47	0.23E-1
4	0	(4413.4255)	-------	----	0.0	4	0	4390.7433	4390.7448(30)	15	0.38E-1
4	1	4413.5098	4413.5104(500)	6	0.18E-1	4	1	4390.6711	4390.6667(500)	-43	0.19E-1
4	2	4413.7678	4413.7682(30)	5	0.16E-1	4	2	4390.4518	4390.4518(30)	0	0.17E-1
4	3	4414.2147	4414.2096(50)	-50	0.28E-1	4	3	4390.0759	4390.0768(30)	10	0.29E-1
4	4	4414.8741	4414.8776(500)	35	0.88E-2	4	4	4389.5282	4389.5300(30)	17	0.92E-2
5	0	4430.9235	4430.9206(30)	-29	0.27E-1	5	0	(4409.5242)	-------	----	0.0
5	1	4431.0013	4430.9987(30)	-25	0.13E-1	5	1	4409.4562	4409.4635(50)	73	0.14E-1
5	2	4431.2398	4431.2370(50)	-27	0.13E-1	5	2	4409.2512	4409.2487(30)	-24	0.13E-1
5	3	4431.6538	4431.6588(50)	50	0.24E-1	5	3	4408.9035	4408.9010(30)	-24	0.25E-1
5	4	4432.2738	4432.2682(30)	-55	0.10E-1	5	4	4408.3986	4408.3971(500)	-14	0.10E-1
5	5	4433.1325	4433.1315(500)	-9	0.65E-2	5	5	4407.7177	4407.7175(500)	-2	0.68E-2
6	0	(4448.0986)	-------	----	0.0	6	0	4428.0689	4428.0690(20)	1	0.18E-1
6	1	4448.1670	4448.1627(30)	-42	0.88E-2	6	1	4428.0038	4428.0026(20)	-12	0.92E-2
6	2	4448.3778	4448.3776(500)	-2	0.87E-2	6	2	4427.8099	4427.8073(50)	-25	0.91E-2
6	3	4448.7491	4448.7487(30)	-3	0.17E-1	6	3	4427.4810	4427.4791(30)	-17	0.18E-1
6	4	4449.3038	4449.3072(50)	35	0.80E-2	6	4	4427.0205	4427.0143(500)	-61	0.83E-2
6	5	4450.0902	4450.0885(50)	-16	0.68E-2	6	5	4426.4064	4426.3971(500)	-92	0.71E-2
6	6	4451.1548	4451.1510(30)	-37	0.90E-2	6	6	4425.6049	4425.3737(30)[a]	-2311	0.94E-2
7	0	4465.0413	4465.0377(100)	-35	0.10E-1	7	0	(4446.3950)	-------	----	0.0
7	1	4465.0972	4465.0963(30)	-8	0.52E-2	7	1	4446.3314	4446.3346(100)	32	0.54E-2
7	2	4465.2701	4465.2682(30)	-19	0.52E-2	7	2	4446.1453	4446.1471(50)	18	0.54E-2
7	3	4465.5689	4465.5807(50)[a]	118	0.10E-1	7	3	4445.8437	4445.8424(30)	-12	0.11E-1
7	4	4466.0429	4466.0377(100)	-51	0.51E-2	7	4	4445.4108	4445.4362(50)[a]	254	0.54E-2
7	5	4466.7200	4466.7174(50)	-25	0.49E-2	7	5	4444.8634	4444.8658(50)	24	0.51E-2
7	6	4467.6657	4467.6627(30)	-29	0.86E-2	7	6	4444.1723	4444.1158(50)[a]	-563	0.90E-2
7	7	4468.9424	4468.9439(30)	15	0.29E-2	7	7	4443.2619	4443.2096(30)[a]	-522	0.30E-2
8	0	(4481.9155)	-------	----	0.0	8	0	4464.5540	4464.5533(50)[a]	-6	0.56E-2
8	1	4481.9547	4481.9557(30)	10	0.27E-2	8	1	4464.4904	4464.4908(30)	5	0.28E-2
8	2	4482.0772	4482.0767(30)	-4	0.27E-2	8	2	4464.3097	4464.3033(50)	-63	0.29E-2
8	3	4482.3057	4482.2799(30)[a]	-257	0.56E-2	8	3	4464.0041	4463.9596(50)[a]	-445	0.59E-2
8	4	4482.6397	4482.6353(30)	-42	0.29E-2	8	4	4463.6263	4463.4947(30)[a]	-1314	0.30E-2
8	5	4483.1596	4483.1588(50)	-7	0.29E-2	8	5	4463.1496	4462.8658(500)[a]	-2837	0.30E-2
8	6	4483.9229	4483.9205(100)	-23	0.57E-2	8	6	4462.5821	4462.1979(100)[a]	-3842	0.59E-2
8	7	4485.0123	4484.9478(50)[a]	-643	0.26E-2	8	7	4461.8697	4461.6471(50)[a]	-2225	0.27E-2
8	8	4486.5026	4486.5338(50)[a]	311	0.18E-2	8	8	4460.8495	4459.9166(100)[a]	-9328	0.19E-2
9	0	4499.0050	4499.0728(100)[a]	678	0.25E-2						
9	1	4499.0223	4498.6705(100)[a]	-3517	0.13E-2						
9	2	4499.0789	4499.0728(100)[a]	-60	0.13E-2						
9	3	4499.1575	4499.2603(30)[a]	1028	0.27E-2						
9	4	4499.3587	4499.4322(30)[a]	735	0.14E-2						
9	5	4499.6605	4499.6744(500)[a]	139	0.15E-2						
9	6	4500.1597	4500.2525(50)[a]	928	0.31E-2						
9	7	4500.9561	4500.8736(500)[a]	-824	0.15E-2						
9	8	4502.1596	4502.2837(30)[a]	1242	0.14E-2						
9	9	4503.8533	4503.7408(100)[a]	-1124	0.20E-2						

fixed values for the ground and ν_2 rotational energies. The rotational energies have been taken from Ref. (*4*) for $^{14}NH_3$ and from Ref. (*6*) for $^{15}NH_3$, respectively. The corresponding molecular parameters are listed in Table V.

A brief inspection of Tables I–IV reveals that the calculated wavenumbers are in close agreement with experimental values for quantum numbers $J < 8$. For higher values of the quantum number J, the parametrization model used in this analysis breaks down because of drastic perturbations of the $\nu_1 + \nu_2$ state arising probably due

TABLE II

Transition Wavenumbers (cm^{-1}) and Intensities (cm^{-2} atm^{-1}) of the $\nu_1 + \nu_2 - \nu_2$ Band of $^{14}NH_3$

sP(J,K)						aP(J,K)					
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
1	0	3367.4601	3367.4658(30)	57	0.19E-1	1	0	(3306.6100)	-------	----	0.0
2	0	(3346.7105)	-------	----	0.0	2	0	3286.8240	3286.8247(20)	7	0.26E-1
2	1	3347.0508	3347.0393(50)[a]	-114	0.12E-1	2	1	3286.7413	3286.7415(20)	2	0.99E-2
3	0	3325.3908	3325.3921(50)	13	0.35E-1	3	0	(3267.0408)	-------	----	0.0
3	1	3325.7181	3325.7195(500)	13	0.16E-1	3	1	3266.9586	3266.9578(30)	-7	0.13E-1
3	2	3326.7182	3326.7197(30)	15	0.10E-1	3	2	3266.7055	3266.7020(30)	-34	0.87E-2
4	0	(3303.5470)	-------	----	0.0	4	0	3247.2674	3247.2694(30)	20	0.27E-1
4	1	3303.8646	3303.8640(500)	-5	0.15E-1	4	1	3247.1869	3247.1861(20)	-7	0.13E-1
4	2	3304.8246	3304.8167(500)[a]	-79	0.13E-1	4	2	3246.9392	3246.9420(50)	28	0.11E-1
4	3	3306.4613	3306.4600(500)	-13	0.16E-1	4	3	3246.5055	3246.5074(20)	19	0.13E-1
5	0	3281.2547	3281.2583(30)	37	0.24E-1	5	0	(3227.5080)	-------	----	0.0
5	1	3281.5568	3281.5559(30)	-8	0.12E-1	5	1	3227.4297	3227.4322(30)	25	0.10E-1
5	2	3282.4682	3282.4668(50)	-13	0.11E-1	5	2	3227.1894	3227.1881(50)	-12	0.92E-2
5	3	3284.0241	3284.0266(30)	25	0.18E-1	5	3	3226.7726	3226.7713(20)	-12	0.15E-1
5	4	3286.2800	3286.2830(50)	30	0.58E-2	5	4	3226.1424	3226.1402(50)	-21	0.48E-2
6	0	(3258.5890)	-------	----	0.0	6	0	3207.7664	3207.7677(20)	13	0.14E-1
6	1	3258.8735	3258.8670(500)	-64	0.80E-2	6	1	3207.6904	3207.6903(30)	0	0.68E-2
6	2	3259.7275	3259.7303(50)	28	0.77E-2	6	2	3207.4579	3207.4581(20)	2	0.66E-2
6	3	3261.1887	3261.1888(30)	1	0.14E-1	6	3	3207.0541	3207.0533(30)	-6	0.12E-1
6	4	3263.3119	3263.3143(50)	23	0.60E-2	6	4	3206.4553	3206.4579(20)	26	0.50E-2
6	5	3266.1753	3266.1780(30)	27	0.39E-2	6	5	3205.6155	3205.6185(50)	30	0.32E-2
7	0	3235.6445	3235.6422(500)	-22	0.96E-2	7	0	(3188.0505)	-------	----	0.0
7	1	3235.9088	3235.9100(30)	12	0.48E-2	7	1	3187.9762	3187.9723(100)	-38	0.41E-2
7	2	3236.6960	3236.6900(500)	-58	0.47E-2	7	2	3187.7502	3187.7519(500)	16	0.41E-2
7	3	3238.0438	3238.0474(30)	37	0.92E-2	7	3	3187.3706	3187.3710(20)	4	0.79E-2
7	4	3240.0145	3240.0181(50)	36	0.43E-2	7	4	3186.7922	3186.7934(30)	12	0.36E-2
7	5	3242.6834	3242.6854(50)	20	0.37E-2	7	5	3186.0019	3186.0016(30)	-2	0.31E-2
7	6	3246.1493	3246.1502(30)	9	0.48E-2	7	6	3184.9264	3184.9240(50)	-23	0.40E-2
8	0	(3212.5393)	-------	----	0.0	8	0	3168.3783	3168.3791(30)	8	0.44E-2
8	1	3212.7812	3212.7865(500)	53	0.25E-2	8	1	3168.3047	3168.3075(100)	29	0.22E-2
8	2	3213.4911	3213.4891(50)	-19	0.25E-2	8	2	3168.0828	3168.0873(50)	45	0.22E-2
8	3	3214.7152	3214.7096(30)	-56	0.51E-2	8	3	3167.7035	3167.7004(50)	-30	0.44E-2
8	4	3216.5004	3216.4957(500)	-46	0.25E-2	8	4	3167.1659	3167.1645(500)	-13	0.22E-2
8	5	3218.9401	3218.9425(50)	23	0.24E-2	8	5	3166.4269	3166.4323(500)	54	0.20E-2
8	6	3222.1364	3222.1336(50)	-27	0.42E-2	8	6	3165.4392	3165.2118(50)[a]	-2272	0.35E-2
8	7	3226.2047	-------	----	0.14E-2	8	7	3164.0858	-------	----	0.12E-2
9	0	3189.4334	3189.4367(50)	33	0.24E-2	9	0	(3148.7878)	-------	----	0.0
9	1	3189.6501	-------	----	0.12E-2	9	1	3148.7135	-------	----	0.11E-2
9	2	3190.2710	3190.2702(100)	-8	0.12E-2	9	2	3148.4925	-------	----	0.11E-2
9	3	3191.3344	3191.3419(100)[a]	76	0.25E-2	9	3	3148.1514	3148.1550(100)	35	0.22E-2
9	4	3192.9211	-------	----	0.13E-2	9	4	3147.6126	-------	----	0.11E-2
9	5	3195.0908	-------	----	0.13E-2	9	5	3146.9268	-------	----	0.11E-2
9	6	3197.9641	3197.9623(500)	-17	0.25E-2	9	6	3146.0363	-------	----	0.21E-2
9	7	3201.6730	-------	----	0.11E-2	9	7	3144.8426	-------	----	0.94E-3
9	8	3206.3454	-------	----	0.78E-3	9	8	3143.1277	-------	----	0.64E-3
10	0	(3166.5571)	-------	----	0.0	10	0	3129.3504	-------	----	0.92E-3
10	1	3166.7459	-------	----	0.52E-3	10	1	3129.2741	-------	----	0.46E-3
10	2	3167.2638	-------	----	0.53E-3	10	2	3129.0507	-------	----	0.47E-3
10	3	3168.1777	-------	----	0.11E-2	10	3	3128.6770	-------	----	0.97E-3
10	4	3169.4958	-------	----	0.57E-3	10	4	3128.2074	-------	----	0.50E-3
10	5	3171.3460	-------	----	0.59E-3	10	5	3127.5804	-------	----	0.52E-3
10	6	3173.8306	-------	----	0.12E-2	10	6	3126.8021	-------	----	0.11E-2
10	7	3177.0966	-------	----	0.61E-3	10	7	3125.7975	-------	----	0.52E-3
10	8	3181.3021	-------	----	0.56E-3	10	8	3124.3760	-------	----	0.47E-3
10	9	3186.5766	-------	----	0.80E-3	10	9	3122.1312	-------	----	0.66E-3
11	0	3144.2576	-------	----	0.40E-3						
11	1	3144.4160	-------	----	0.20E-3						
11	2	3144.8134	-------	----	0.20E-3						
11	3	3145.4819	-------	----	0.43E-3						
11	4	3146.5561	-------	----	0.22E-3						
11	5	3148.0266	-------	----	0.24E-3						
11	6	3150.0413	-------	----	0.51E-3						
11	7	3152.7592	-------	----	0.27E-3						
11	8	3156.3665	-------	----	0.28E-3						
11	9	3161.0441	-------	----	0.53E-3						
11	10	3166.9045	-------	----	0.20E-3						

[a] Lines not used in the least squares fit in obtaining molecular parameters.

TABLE II—*Continued*

sQ(J,K)						aQ(J,K)					
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
0	0	(3387.5959)	-------	----	0.0	0	0	(3326.3872)	-------	----	0.0
1	0	(3386.9551)	-------	----	0.0	1	0	(3326.3618)	-------	----	0.0
1	1	3387.3050	3387.3031(20)	-18	0.15E-1	1	1	3326.2840	3326.2851(50)	12	0.12E-1
2	0	(3385.6882)	-------	----	0.0	2	0	(3326.3056)	-------	----	0.0
2	1	3386.0322	3386.0348(50)	26	0.68E-2	2	1	3326.2308	3326.2197(500)	-110	0.56E-2
2	2	3387.0755	3387.0768(50)	13	0.29E-1	2	2	3326.0000	3325.9995(30)	-4	0.24E-1
3	0	(3383.8262)	-------	----	0.0	3	0	(3326.2089)	-------	----	0.0
3	1	3384.1589	3384.1654(500)	65	0.35E-2	3	1	3326.1383	-------	----	0.29E-2
3	2	3385.1757	3385.1776(50)	19	0.15E-1	3	2	3325.9203	3325.9219(50)	15	0.12E-1
3	3	3386.9079	3386.9101(30)	21	0.74E-1	3	3	3325.5338	3325.5349(50)	11	0.61E-1
4	0	(3381.4025)	-------	----	0.0	4	0	(3326.0590)	-------	----	0.0
4	1	3381.7270	-------	----	0.19E-2	4	1	3325.9932	-------	----	0.16E-2
4	2	3382.7082	3382.7069(30)	-11	0.78E-2	4	2	3325.7901	3325.7910(50)	9	0.65E-2
4	3	3384.3816	3384.3859(100)	43	0.39E-1	4	3	3325.4329	3325.4338(50)	9	0.32E-1
4	4	3386.8042	3386.8090(500)	48	0.39E-1	4	4	3324.8915	3324.8921(50)	6	0.32E-1
5	0	(3378.4819)	-------	----	0.0	5	0	(3325.8428)	-------	----	0.0
5	1	3378.7921	-------	----	0.93E-3	5	1	3325.7817	-------	----	0.79E-3
5	2	3379.7280	3379.7240(30)	-39	0.39E-2	5	2	3325.5941	-------	----	0.33E-2
5	3	3381.3268	3381.3256(30)	-11	0.19E-1	5	3	3325.2673	3325.2729(30)	57	0.16E-1
5	4	3383.6466	3383.6476(30)	11	0.20E-1	5	4	3324.7696	3324.7671(50)	-25	0.16E-1
5	5	3386.7672	3386.7731(500)	59	0.36E-1	5	5	3324.0636	3324.0644(30)	8	0.29E-1
6	0	(3375.1338)	-------	----	0.0	6	0	(3325.5511)	-------	----	0.0
6	1	3375.4270	-------	----	0.44E-3	6	1	3325.4943	-------	----	0.38E-3
6	2	3376.3075	3376.3127(500)	51	0.19E-2	6	2	3325.3209	-------	----	0.16E-2
6	3	3377.8134	3377.8132(30)	-1	0.91E-2	6	3	3325.0205	3325.0229(30)	25	0.77E-2
6	4	3380.0062	3380.0041(30)	-20	0.92E-2	6	4	3324.5707	3324.5705(500)	0	0.77E-2
6	5	3382.9678	3382.9689(50)	11	0.17E-1	6	5	3323.9368	3323.9336(500)	-32	0.14E-1
6	6	3386.8007	-------	----	0.60E-1	6	6	3323.0520	3323.0525(30)	5	0.49E-1
7	0	(3371.4574)	-------	----	0.0	7	0	(3325.1852)	-------	----	0.0
7	1	3371.7306	-------	----	0.19E-3	7	1	3325.1316	-------	----	0.17E-3
7	2	3372.5447	-------	----	0.82E-3	7	2	3324.9701	-------	----	0.71E-3
7	3	3373.9408	3373.9372(500)	-36	0.40E-2	7	3	3324.6988	-------	----	0.35E-2
7	4	3375.9761	3375.9794(30)	33	0.41E-2	7	4	3324.2903	3324.2846(500)	-55	0.34E-2
7	5	3378.7409	3378.7419(30)	10	0.74E-2	7	5	3323.7304	3323.7312(100)	8	0.63E-2
7	6	3382.3446	3382.3437(50)	-9	0.26E-1	7	6	3322.9612	3322.7368(500)[a]	-2243	0.22E-1
7	7	3386.9093	-------	----	0.23E-1	7	7	3321.8653	3321.8913(100)	260	0.18E-1
8	0	(3367.5955)	-------	----	0.0	8	0	(3324.7665)	-------	----	0.0
8	1	3367.8456	3367.8408(500)	-47	0.80E-4	8	1	3324.7147	-------	----	0.70E-4
8	2	3368.5805	-------	----	0.34E-3	8	2	3324.5621	-------	----	0.29E-3
8	3	3369.8386	-------	----	0.17E-2	8	3	3324.3117	-------	----	0.14E-2
8	4	3371.6904	3371.6869(500)	-34	0.17E-2	8	4	3323.9479	-------	----	0.14E-2
8	5	3374.2141	3374.2172(50)	32	0.30E-2	8	5	3323.4637	-------	----	0.26E-2
8	6	3377.5310	3377.5273(500)	-36	0.11E-1	8	6	3322.8193	3322.7607(500)[a]	-585	0.89E-2
8	7	3381.7804	3381.7841(20)	37	0.91E-2	8	7	3321.9161	3321.8616(500)[a]	-544	0.76E-2
8	8	3387.0989	3387.1005(50)	16	0.16E-1	8	8	3320.5356	3320.5339(500)[a]	-16	0.13E-1
9	0	(3363.7640)	-------	----	0.0	9	0	(3324.3501)	-------	----	0.0
9	1	3363.9874	-------	----	0.30E-4	9	1	3324.2988	-------	----	0.27E-4
9	2	3364.6286	-------	----	0.13E-3	9	2	3324.1522	-------	----	0.11E-3
9	3	3365.7371	-------	----	0.62E-3	9	3	3323.9257	-------	----	0.55E-3
9	4	3367.3534	-------	----	0.63E-3	9	4	3323.6022	-------	----	0.55E-3
9	5	3369.5829	-------	----	0.11E-2	9	5	3323.1989	-------	----	0.99E-3
9	6	3372.5428	3372.5383(100)	-45	0.40E-2	9	6	3322.6940	-------	----	0.34E-2
9	7	3376.3879	3376.3246(30)[a]	-632	0.34E-2	9	7	3322.0126	-------	----	0.29E-2
9	8	3381.2855	-------	----	0.59E-2	9	8	3320.9635	-------	----	0.48E-2
9	9	3387.3765	3387.4399(20)[a]	634	0.20E-1	9	9	3319.1397	-------	----	0.16E-1
10	0	(3360.2978)	-------	----	0.0						
10	1	3360.4907	-------	----	0.11E-4						
10	2	3361.0205	-------	----	0.44E-4						
10	3	3361.9204	-------	----	0.22E-3						
10	4	3363.2844	-------	----	0.22E-3						
10	5	3365.1559	-------	----	0.40E-3						
10	6	3367.6730	-------	----	0.14E-2						
10	7	3371.0027	-------	----	0.12E-2						
10	8	3375.3413	-------	----	0.20E-2						
10	9	3380.8817	3380.7719(30)[a]	-1097	0.69E-2						
10	10	3387.7507	3387.7614(30)[a]	107	0.61E-2						

TABLE II—*Continued*

sR(J,K)						aR(J,K)					
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
0	0	(3407.0910)	-------	----	0.0	0	0	3346.1390	3346.1401(30)	11	0.18E-1
1	0	3425.9328	3425.9357(500)	28	0.39E-1	1	0	(3365.8433)	-------	----	0.0
1	1	3426.2865	3426.2867(20)	2	0.15E-1	1	1	3365.7735	3365.7751(500)[a]	15	0.12E-1
2	0	(3444.1236)	-------	----	0.0	2	0	3385.4737	3385.4753(20)	15	0.40E-1
2	1	3444.4730	3444.4688(50)	-41	0.22E-1	2	1	3385.4105	3385.4098(20)	-6	0.18E-1
2	2	3445.5329	3445.5345(50)	16	0.15E-1	2	2	3385.2148	3385.2074(30)[a]	-73	0.12E-1
3	0	3461.6816	3461.6807(50)	-8	0.49E-1	3	0	(3405.0006)	-------	----	0.0
3	1	3462.0213	3462.0201(50)	-11	0.23E-1	3	1	3404.9446	3404.9494(500)[a]	47	0.19E-1
3	2	3463.0592	3463.0621(20)	29	0.20E-1	3	2	3404.7713	3404.7706(30)	-5	0.16E-1
3	3	3464.8282	3464.8304(30)	22	0.25E-1	3	3	3404.4612	3404.4611(50)	0	0.21E-1
4	0	(3478.6297)	-------	----	0.0	4	0	3424.3939	3424.3937(30)	-1	0.35E-1
4	1	3478.9623	3478.9639(20)	17	0.20E-1	4	1	3424.3452	3424.3461(50)	9	0.17E-1
4	2	3479.9680	3479.9703(50)	23	0.19E-1	4	2	3424.1948	3424.1971(50)	24	0.16E-1
4	3	3481.6843	3481.6849(30)	5	0.31E-1	4	3	3423.9275	3423.9293(30)	18	0.26E-1
4	4	3484.1708	3484.1734(30)	26	0.10E-1	4	4	3423.5187	3423.5184(50)	-2	0.82E-2
5	0	3495.0266	3495.0266(30)	1	0.31E-1	5	0	(3443.6275)	-------	----	0.0
5	1	3495.3455	3495.3482(20)	26	0.15E-1	5	1	3443.5856	3443.5877(20)	21	0.13E-1
5	2	3496.3081	3496.3067(30)	-14	0.15E-1	5	2	3443.4570	3443.4569(30)	-1	0.12E-1
5	3	3497.9515	3497.9500(20)	-14	0.27E-1	5	3	3443.2336	3443.2367(30)	30	0.23E-1
5	4	3500.3408	3500.3372(50)	-35	0.11E-1	5	4	3442.8850	3442.8792(100)	-57	0.95E-2
5	5	3503.5597	3503.5581(20)	-15	0.74E-2	5	5	3442.3849	3442.3912(50)	63	0.61E-2
6	0	(3510.9466)	-------	----	0.0	6	0	3462.6858	3462.6868(50)	10	0.17E-1
6	1	3511.2487	3511.2500(30)	13	0.10E-1	6	1	3462.6497	3462.6512(50)	15	0.87E-2
6	2	3512.1562	3512.1670(500)	107	0.10E-1	6	2	3462.5407	3462.5379(500)[a]	-27	0.86E-2
6	3	3513.7104	3513.7090(50)	-13	0.20E-1	6	3	3462.3487	3462.3475(30)	-11	0.17E-1
6	4	3515.9678	3515.9712(20)	34	0.91E-2	6	4	3462.0688	3462.0677(30)	-10	0.77E-2
6	5	3519.0253	3519.0254(50)	1	0.78E-2	6	5	3461.6653	3461.6509(100)	-142	0.65E-2
6	6	3522.9960	3522.9963(50)	3	0.10E-1	6	6	3461.0868	3460.8590(30)[a]	-2277	0.84E-2
7	0	3526.5135	3526.5149(20)	13	0.12E-1	7	0	(3481.5735)	-------	----	0.0
7	1	3526.7951	3526.7947(500)	-3	0.60E-2	7	1	3481.5417	3481.5418(20)	1	0.52E-2
7	2	3527.6341	3527.6343(50)	2	0.60E-2	7	2	3481.4494	3481.4527(50)	33	0.52E-2
7	3	3529.0642	3529.0749(500)[a]	108	0.12E-1	7	3	3481.3070	3481.3096(30)	26	0.10E-1
7	4	3531.1661	3531.1648(20)	-12	0.59E-2	7	4	3481.0723	3481.1014(50)[a]	291	0.51E-2
7	5	3534.0148	3534.0163(20)	15	0.57E-2	7	5	3480.7672	3480.7679(100)	7	0.48E-2
7	6	3537.7392	3537.7373(20)	-18	0.99E-2	7	6	3480.3413	3480.2857(100)[a]	-555	0.82E-2
7	7	3542.4850	3542.4944(500)	93	0.34E-2	7	7	3479.6956	3479.6487(20)[a]	-468	0.27E-2
8	0	(3541.9261)	-------	----	0.0	8	0	3500.3288	-------	----	0.55E-2
8	1	3542.1830	3542.1848(30)	18	0.32E-2	8	1	3500.3000	3500.3015(30)	15	0.28E-2
8	2	3542.9380	3542.9348(100)	-32	0.32E-2	8	2	3500.2218	3500.2180(30)	-37	0.28E-2
8	3	3544.2413	3544.2207(50)[a]	-205	0.65E-2	8	3	3500.0860	3500.0454(30)[a]	-404	0.57E-2
8	4	3546.1227	3546.1248(30)	21	0.33E-2	8	4	3499.9375	3499.8074(50)[a]	-1300	0.29E-2
8	5	3548.7062	3548.4360(500)[a]	-2701	0.34E-2	8	5	3499.7358	3499.4561(50)[a]	-2796	0.29E-2
8	6	3552.1098	3552.1032(500)	-65	0.66E-2	8	6	3499.4771	3499.0989(30)[a]	-3781	0.55E-2
8	7	3556.4953	3556.4316(30)[a]	-636	0.30E-2	8	7	3499.0861	-------	----	0.24E-2
8	8	3562.0390	3562.0754(30)[a]	364	0.21E-2	8	8	3498.3714	-------	----	0.17E-2
9	0	3557.5047	3557.5747(30)[a]	700	0.30E-2						
9	1	3557.7321	3557.3723(500)[a]	-3598	0.15E-2						
9	2	3558.3852	3558.3842(30)[a]	-9	0.15E-2						
9	3	3559.4799	3559.5810(30)[a]	1011	0.32E-2						
9	4	3561.1420	3561.2182(100)[a]	762	0.16E-2						
9	5	3563.3928	3563.4150(500)[a]	222	0.17E-2						
9	6	3566.3852	-------	----	0.36E-2						
9	7	3570.2940	3570.2079(50)[a]	-859	0.18E-2						
9	8	3575.3247	-------	----	0.17E-2						
9	9	3581.6816	3581.5673(50)[a]	-1142	0.24E-2						

to interlevel crossing with the $\nu_2 + 2\nu_4$ vibrational state. These resonance perturbations are obviously the reason for a relatively poor determination of the higher-order centrifugal distortion constants. On the other hand, the elimination of the octic constants has already led to a breakdown of the model for the $\nu_1 + \nu_2$ energy levels with quantum numbers $J > 5$.

The complexity of the $\nu_1 + \nu_2$ state, in combination with significantly lower resolution, could have caused some problems in the previous analysis (*1*). No surprise

TABLE III

Transition Wavenumbers (cm^{-1}) and Intensities (cm^{-2} atm^{-1}) of the $\nu_1 + \nu_2$ Band of $^{15}NH_3$

			sP(J,K)						aP(J,K)		
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
1	0	4292.4627	4292.4616(20)	-9	0.17E-1	1	0	(4267.4352)	-------	----	0.0
2	0	(4272.2511)	-------	----	0.0	2	0	4247.4930	4247.4932(20)	2	0.29E-1
2	1	4272.3319	4272.3306(50)	-12	0.11E-1	2	1	4247.3947	4247.3963(30)	16	0.11E-1
3	0	4251.6965	4251.6960(20)	-4	0.31E-1	3	0	(4227.4572)	-------	----	0.0
3	1	4251.7717	4251.7725(20)	8	0.14E-1	3	1	4227.3575	4227.3562(20)	-12	0.15E-1
3	2	4252.0013	4252.0017(30)	4	0.93E-2	3	2	4227.0543	4227.0541(20)	-2	0.97E-2
4	0	(4230.8321)	-------	----	0.0	4	0	4207.3425	4207.3417(20)	-6	0.29E-1
4	1	4230.9005	4230.8999(20)	-5	0.13E-1	4	1	4207.2422	4207.2413(20)	-9	0.14E-1
4	2	4231.1098	4231.1107(30)	10	0.11E-1	4	2	4206.9375	4206.9379(20)	4	0.12E-1
4	3	4231.4723	4231.4731(30)	8	0.14E-1	4	3	4206.4158	4206.4143(20)	-14	0.15E-1
5	0	4209.6977	4209.6988(20)	10	0.21E-1	5	0	(4187.1625)	-------	----	0.0
5	1	4209.7580	4209.7567(30)	-12	0.11E-1	5	1	4187.0622	4187.0615(30)	-6	0.11E-1
5	2	4209.9431	4209.9447(20)	15	0.97E-2	5	2	4186.7576	4186.7570(30)	-5	0.10E-1
5	3	4210.2658	4210.2650(20)	-8	0.16E-1	5	3	4186.2372	4186.2371(20)	0	0.17E-1
5	4	4210.7472	4210.7450(30)	-21	0.52E-2	5	4	4185.4799	4185.4755(30)	-42	0.54E-2
6	0	(4188.3405)	-------	----	0.0	6	0	4166.9321	4166.9331(30)	10	0.15E-1
6	1	4188.3911	4188.3928(30)	17	0.71E-2	6	1	4166.8319	4166.8310(500)	-8	0.74E-2
6	2	4188.5477	4188.5497(30)	20	0.69E-2	6	2	4166.5282	4166.5292(50)	10	0.71E-2
6	3	4188.8241	4188.8240(30)	0	0.13E-1	6	3	4166.0098	4166.0068(30)	-29	0.13E-1
6	4	4189.2410	4189.2390(30)	-18	0.53E-2	6	4	4165.2605	4165.2616(100)	11	0.55E-2
6	5	4189.8311	4189.8232(30)[a]	-78	0.34E-2	6	5	4164.2479	4164.2451(30)	-27	0.36E-2
7	0	4166.8187	4166.8258(500)	71	0.85E-2	7	0	(4146.6705)	-------	----	0.0
7	1	4166.8578	4166.8584(50)	6	0.42E-2	7	1	4146.5700	4146.5693(30)	-6	0.44E-2
7	2	4166.9803	4166.9795(50)	-7	0.42E-2	7	2	4146.2664	4146.2646(30)	-16	0.44E-2
7	3	4167.1992	4167.2001(30)	8	0.81E-2	7	3	4145.7518	4145.7541(50)	23	0.85E-2
7	4	4167.5414	4167.5381(30)	-32	0.38E-2	7	4	4145.0080	4145.0068(30)	-11	0.40E-2
7	5	4168.0357	4168.0381(100)	24	0.32E-2	7	5	4144.0156	4144.0146(30)	-9	0.34E-2
7	6	4168.7348	4168.7138(50)[a]	-208	0.43E-2	7	6	4142.7261	4142.7264(100)	3	0.45E-2
8	0	(4145.2092)	-------	----	0.0	8	0	4126.4056	4126.4053(30)	-2	0.47E-2
8	1	4145.2343	4145.2334(30)	-8	0.22E-2	8	1	4126.3036	4126.3037(30)	1	0.23E-2
8	2	4145.3154	4145.3115(30)	-38	0.22E-2	8	2	4125.9974	4125.9951(30)	-22	0.23E-2
8	3	4145.4697	4145.4678(30)	-19	0.45E-2	8	3	4125.4762	4125.4717(30)	-44	0.47E-2
8	4	4145.7154	4145.7139(50)	-15	0.22E-2	8	4	4124.7398	4124.7373(20)	-23	0.23E-2
8	5	4146.0930	4146.0928(20)	-1	0.21E-2	8	5	4123.7646	4123.7608(30)	-38	0.22E-2
8	6	4146.6514	4146.6499(50)	-14	0.37E-2	8	6	4122.5224	4122.5381(30)[a]	157	0.38E-2
8	7	4147.4828	4147.4053(20)[a]	-773	0.12E-2	8	7	4120.9343	4120.9053(30)[a]	-289	0.13E-2
9	0	4123.6220	4123.6201(50)	-17	0.21E-2	9	0	(4106.1800)	-------	----	0.0
9	1	4123.6297	4123.6236(100)	-60	0.11E-2	9	1	4106.0743	4106.0694(50)	-48	0.11E-2
9	2	4123.6593	4123.6592(50)	0	0.11E-2	9	2	4105.7599	4105.7569(20)	-29	0.11E-2
9	3	4123.7202	4123.7217(30)	15	0.22E-2	9	3	4105.2369	4105.2344(500)	-24	0.23E-2
9	4	4123.8574	4123.8545(20)	-28	0.11E-2	9	4	4104.4836	4104.5025(500)	189	0.12E-2
9	5	4124.0886	4124.0850(20)	-36	0.11E-2	9	5	4103.5153	4103.5147(20)	-5	0.12E-2
9	6	4124.4706	4124.4717(30)	11	0.22E-2	9	6	4102.3134	4102.5889(30)[a]	2755	0.23E-2
9	7	4125.0924	4125.0928(20)	4	0.99E-3	9	7	4100.8296	4100.7530(30)[a]	-765	0.10E-2
9	8	4126.1266	4125.9170(20)[a]	-2095	0.69E-3	9	8	4098.9226	4098.9209(30)	-15	0.71E-3
10	0	(4102.2229)	-------	----	0.0	10	0	4086.0586	4086.0528(30)	-57	0.93E-3
10	1	4102.2082	4102.2061(100)	-20	0.45E-3	10	1	4085.9453	4085.9522(30)	69	0.47E-3
10	2	4102.1720	4102.1748(100)	29	0.46E-3	10	2	4085.6137	4085.6168(30)[a]	31	0.48E-3
10	3	4102.1379	4102.1358(100)	-20	0.95E-3	10	3	4085.0468	4085.0442(30)	-25	0.99E-3
10	4	4102.1101	-------	----	0.49E-3	10	4	4084.2845	4084.1133(20)[a]	-1710	0.52E-3
10	5	4102.1524	4102.1490(500)[a]	-32	0.52E-3	10	5	4083.3021	4083.4649(30)[a]	1628	0.54E-3
10	6	4102.3063	4102.2764(30)[a]	-298	0.11E-2	10	6	4082.1217	4082.0565(20)[a]	-651	0.11E-2
10	7	4102.6579	4101.9795(30)[a]	-6782	0.54E-3	10	7	4080.7305	-------	----	0.56E-3
10	8	4103.3714	4103.3702(20)	-11	0.49E-3	10	8	4079.0413	-------	----	0.51E-3
10	9	4104.7672	4104.2686(100)[a]	-4985	0.71E-3	10	9	4076.7975	4076.0987(30)[a]	-6987	0.74E-3
11	0	4081.2685	-------	----	0.34E-3						
11	1	4081.2246	4081.2852(20)[a]	606	0.17E-3						
11	2	4081.1025	4081.1790(50)[a]	765	0.18E-3						
11	3	4080.8949	4081.0059(30)[a]	1110	0.37E-3						
11	4	4080.6975	4080.7935(100)[a]	961	0.19E-3						
11	5	4080.4899	4080.5811(30)[a]	912	0.21E-3						
11	6	4080.3419	4080.3463(30)[a]	44	0.45E-3						
11	7	4080.3361	-------	----	0.24E-3						
11	8	4080.6278	4081.4642(50)[a]	8364	0.24E-3						
11	9	4081.5206	4081.3467(50)[a]	-1738	0.46E-3						
11	10	4083.5894	4082.3975(50)[a]	-11918	0.17E-3						

[a] Lines not used in the least squares fit in obtaining molecular parameters.

TABLE III—*Continued*

		sQ(J,K)						aQ(J,K)			
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
0	0	(4312.3040)	-------	----	0.0	0	0	(4287.2668)	-------	----	0.0
1	0	(4311.9133)	-------	----	0.0	1	0	(4287.1360)	-------	----	0.0
1	1	4312.0004	4312.0003(20)	0	0.13E-1	1	1	4287.0438	4287.0455(30)	17	0.14E-1
2	0	(4311.1390)	-------	----	0.0	2	0	(4286.8719)	-------	----	0.0
2	1	4311.2236	4311.2240(30)	4	0.60E-2	2	1	4286.7814	4286.7827(50)	13	0.62E-2
2	2	4311.4815	4311.4812(20)	-2	0.25E-1	2	2	4286.5057	4286.5050(30)	-6	0.26E-1
3	0	(4309.9944)	-------	----	0.0	3	0	(4286.4694)	-------	----	0.0
3	1	4310.0753	4310.0777(50)	25	0.31E-2	3	1	4286.3813	4286.3817(30)	4	0.33E-2
3	2	4310.3220	4310.3230(500)	10	0.13E-1	3	2	4286.1130	4286.1179(50)	48	0.14E-1
3	3	4310.7473	4310.7501(30)	28	0.65E-1	3	3	4285.6524	4285.6542(20)	17	0.68E-1
4	0	(4308.5002)	-------	----	0.0	4	0	(4285.9233)	-------	----	0.0
4	1	4308.5758	4308.5730(30)	-27	0.16E-2	4	1	4285.8380	4285.8387(20)	7	0.17E-2
4	2	4308.8073	4308.8058(50)	-14	0.69E-2	4	2	4285.5786	4285.5770(30)	-15	0.72E-2
4	3	4309.2078	4309.2074(20)	-4	0.34E-1	4	3	4285.1337	4285.1345(30)	8	0.35E-1
4	4	4309.7988	4309.7986(20)	-1	0.34E-1	4	4	4284.4831	4284.4825(100)	-6	0.36E-1
5	0	(4306.6847)	-------	----	0.0	5	0	(4285.2299)	-------	----	0.0
5	1	4306.7536	4306.7488(20)	-47	0.82E-3	5	1	4285.1475	4285.1434(500)	-40	0.86E-3
5	2	4306.9651	4306.9637(500)	-13	0.35E-2	5	2	4284.8974	4284.9012(30)	38	0.36E-2
5	3	4307.3330	4307.3338(20)	8	0.17E-1	5	3	4284.4692	4284.4637(500)	-54	0.18E-1
5	4	4307.8803	4307.8810(20)	8	0.17E-1	5	4	4283.8460	4283.8485(30)	25	0.18E-1
5	5	4308.6394	4308.6326(100)[a]	-67	0.32E-1	5	5	4282.9977	4282.9990(30)	13	0.33E-1
6	0	(4304.5886)	-------	----	0.0	6	0	(4284.3907)	-------	----	0.0
6	1	4304.6487	4304.6434(50)	-52	0.39E-3	6	1	4284.3107	4284.3074(30)	-32	0.40E-3
6	2	4304.8343	4304.8348(30)	5	0.16E-2	6	2	4284.0688	4284.0653(100)	-35	0.17E-2
6	3	4305.1601	4305.1605(20)	4	0.80E-2	6	3	4283.6563	4283.6541(100)	-20	0.84E-2
6	4	4305.6504	4305.6434(500)	-69	0.81E-2	6	4	4283.0595	4283.0535(500)	-58	0.85E-2
6	5	4306.3388	4306.3388(30)	0	0.15E-1	6	5	4282.2562	4282.2575(30)	13	0.16E-1
6	6	4307.2787	4307.2572(20)[a]	-214	0.52E-1	6	6	4281.2008	4281.2011(20)	3	0.55E-1
7	0	(4302.2720)	-------	----	0.0	7	0	(4283.4169)	-------	----	0.0
7	1	4302.3207	4302.3270(500)	63	0.17E-3	7	1	4283.3380	4283.3348(50)	-32	0.18E-3
7	2	4302.4726	4302.4715(30)	-11	0.72E-3	7	2	4283.1013	4283.1011(500)	-1	0.75E-3
7	3	4302.7430	4302.7410(30)	-19	0.35E-2	7	3	4282.6992	4282.6990(30)	-1	0.37E-2
7	4	4303.1591	4303.1590(20)	0	0.36E-2	7	4	4282.1239	4282.1199(30)	-38	0.37E-2
7	5	4303.7546	4303.7566(30)	20	0.65E-2	7	5	4281.3616	4281.3617(30)	1	0.68E-2
7	6	4304.5833	4304.5834(20)	1	0.23E-1	7	6	4280.3829	4280.3963(20)[a]	134	0.24E-1
7	7	4305.7398	4305.6632(50)[a]	-764	0.20E-1	7	7	4279.1107	4279.0863(20)[a]	-243	0.21E-1
8	0	(4299.8290)	-------	----	0.0	8	0	(4282.3353)	-------	----	0.0
8	1	4299.8627	-------	----	0.69E-4	8	1	4282.2551	-------	----	0.73E-4
8	2	4299.9705	4299.9676(500)[a]	-28	0.29E-3	8	2	4282.0175	4282.0106(100)	-68	0.31E-3
8	3	4300.1681	4300.1702(120)	21	0.14E-2	8	3	4281.6173	4281.6239(30)	66	0.15E-2
8	4	4300.4847	4300.4832(50)	-14	0.14E-2	8	4	4281.0511	4281.0653(30)[a]	142	0.15E-2
8	5	4300.9564	4300.9559(20)	-5	0.27E-2	8	5	4280.3181	4280.3192(50)	11	0.28E-2
8	6	4301.6364	4301.6349(20)	-14	0.93E-2	8	6	4279.4075	4279.6847(30)[a]	2772	0.97E-2
8	7	4302.6166	4302.6164(30)	-2	0.80E-2	8	7	4278.2729	4278.2034(30)[a]	-694	0.83E-2
8	8	4304.0728	4303.8635(30)[a]	-2093	0.14E-1	8	8	4276.7758	4276.7787(30)	29	0.14E-1
9	0	(4297.4108)	-------	----	0.0	9	0	(4281.1958)	-------	----	0.0
9	1	4297.4245	-------	----	0.26E-4	9	1	4281.1103	-------	----	0.27E-4
9	2	4297.4734	-------	----	0.11E-3	9	2	4280.8624	-------	----	0.12E-3
9	3	4297.5715	4297.5691(100)	-22	0.54E-3	9	3	4280.4464	4280.4364(100)	-99	0.56E-3
9	4	4297.7553	-------	----	0.54E-3	9	4	4279.8710	-------	----	0.57E-3
9	5	4298.0591	4298.0613(30)	22	0.99E-3	9	5	4279.1452	4279.3099(30)[a]	1647	0.10E-2
9	6	4298.5370	4298.5145(30)[a]	-225	0.35E-2	9	6	4278.2821	-------	----	0.36E-2
9	7	4299.2780	4298.6043(30)[a]	-6736	0.30E-2	9	7	4277.2714	4276.8621(100)[a]	-4092	0.31E-2
9	8	4300.4498	4300.4520(50)	21	0.51E-2	9	8	4276.0289	4275.4246(100)[a]	-6041	0.53E-2
9	9	4302.3775	4301.8752(20)[a]	-5021	0.18E-1	9	9	4274.3014	4273.5996(20)[a]	-7017	0.18E-1
10	0	(4295.2607)	-------	----	0.0						
10	1	4295.2472	-------	----	0.90E-5						
10	2	4295.2166	-------	----	0.38E-4						
10	3	4295.1806	-------	----	0.19E-3						
10	4	4295.1812	4295.2723(100)[a]	911	0.19E-3						
10	5	4295.2548	4295.3387(50)[a]	839	0.34E-3						
10	6	4295.4548	4295.4559(50)[a]	10	0.12E-2						
10	7	4295.8671	-------	----	0.10E-2						
10	8	4296.6508	4297.4871(30)[a]	8363	0.18E-2						
10	9	4298.1139	4297.9440(30)[a]	-1698	0.60E-2						
10	10	4300.8372	4299.6395(30)[a]	-11976	0.53E-2						

TABLE III—*Continued*

sR(J,K)						aR(J,K)					
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
0	0	(4331.7546)	-------	----	0.0	0	0	4306.9676	4306.9668(30)	-7	0.20E-1
1	0	4350.8012	4350.8008(20)	-3	0.35E-1	1	0	(4326.5149)	-------	----	0.0
1	1	4350.8921	4350.8933(500)	12	0.13E-1	1	1	4326.4305	4326.4314(100)	9	0.14E-1
2	0	(4369.4369)	-------	----	0.0	2	0	4345.8841	4345.8831(20)	-8	0.45E-1
2	1	4369.5272	4369.5285(20)	13	0.19E-1	2	1	4345.8051	4345.8046(20)	-5	0.20E-1
2	2	4369.8023	4369.8028(20)	5	0.13E-1	2	2	4345.5644	4345.5638(20)	-5	0.13E-1
3	0	4387.6625	4387.6615(20)	-8	0.43E-1	3	0	(4365.0502)	-------	----	0.0
3	1	4387.7506	4387.7503(20)	-2	0.21E-1	3	1	4364.9771	4364.9787(30)	17	0.21E-1
3	2	4388.0195	4388.0190(30)	-4	0.17E-1	3	2	4364.7541	4364.7553(30)	12	0.18E-1
3	3	4388.4829	4388.4753(500)	-75	0.22E-1	3	3	4364.3703	4364.3710(100)	7	0.23E-1
4	0	(4405.4872)	-------	----	0.0	4	0	4383.9907	4383.9933(30)	26	0.38E-1
4	1	4405.5714	4405.5725(30)	11	0.18E-1	4	1	4383.9233	4383.9258(100)	25	0.19E-1
4	2	4405.8292	4405.8299(20)	7	0.16E-1	4	2	4383.7183	4383.7196(20)	13	0.17E-1
4	3	4406.2750	4406.2762(30)	12	0.28E-1	4	3	4383.3657	4383.3701(500)	44	0.29E-1
4	4	4406.9319	4406.9315(30)	-2	0.88E-2	4	4	4382.8493	4382.8525(30)	33	0.92E-2
5	0	4422.9328	4422.9333(30)	5	0.27E-1	5	0	(4402.6885)	-------	----	0.0
5	1	4423.0111	4423.0116(20)	4	0.13E-1	5	1	4402.6263	4402.6249(30)	-14	0.14E-1
5	2	4423.2516	4423.2518(20)	2	0.13E-1	5	2	4402.4380	4402.4383(30)	3	0.14E-1
5	3	4423.6690	4423.6701(20)	11	0.24E-1	5	3	4402.1157	4402.1181(30)	24	0.25E-1
5	4	4424.2897	4424.2877(100)	-18	0.10E-1	5	4	4401.6449	4401.6455(30)	6	0.10E-1
5	5	4425.1471	4425.1460(500)	-10	0.65E-2	5	5	4401.0060	4401.0071(50)	11	0.68E-2
6	0	(4440.0419)	-------	----	0.0	6	0	4421.1372	4421.1354(500)	-17	0.19E-1
6	1	4440.1115	4440.1134(30)	18	0.89E-2	6	1	4421.0788	4421.0815(20)	27	0.92E-2
6	2	4440.3266	4440.3266(20)	0	0.88E-2	6	2	4420.9037	4420.9010(50)	-26	0.91E-2
6	3	4440.7039	4440.7013(20)	-25	0.17E-1	6	3	4420.6037	4420.6018(20)	-17	0.18E-1
6	4	4441.2680	4441.2692(20)	12	0.80E-2	6	4	4420.1753	4420.1769(30)	16	0.83E-2
6	5	4442.0578	4442.0591(20)	13	0.68E-2	6	5	4419.6022	4419.6018(30)	-3	0.71E-2
6	6	4443.1273	4443.1263(20)	-9	0.90E-2	6	6	4418.8576	4418.8709(30)[a]	133	0.94E-2
7	0	4456.8917	4456.8921(20)	3	0.10E-1	7	0	(4439.3467)	-------	----	0.0
7	1	4456.9490	4456.9485(30)	-5	0.52E-2	7	1	4439.2895	4439.2885(30)	-10	0.54E-2
7	2	4457.1277	4457.1268(30)	-8	0.52E-2	7	2	4439.1214	4439.1198(30)	-14	0.54E-2
7	3	4457.4413	4457.4450(30)	37	0.10E-1	7	3	4438.8402	4438.8455(20)	52	0.11E-1
7	4	4457.9283	4457.9261(30)	-22	0.52E-2	7	4	4438.4352	4438.4479(30)[a]	128	0.54E-2
7	5	4458.6181	4458.6185(30)	4	0.49E-2	7	5	4437.9151	4437.9166(50)	15	0.51E-2
7	6	4459.5684	4459.5688(20)	4	0.86E-2	7	6	4437.2679	4437.5432(30)[a]	2753	0.90E-2
7	7	4460.8737	4460.8718(50)	-17	0.29E-2	7	7	4436.4492	4436.3737(500)[a]	-755	0.30E-2
8	0	(4473.6178)	-------	----	0.0	8	0	4457.3511	4457.3502(30)	-8	0.57E-2
8	1	4473.6575	4473.6602(30)	27	0.27E-2	8	1	4457.2911	4457.2955(30)	44	0.28E-2
8	2	4473.7846	4473.7838(20)	-7	0.28E-2	8	2	4457.1200	4457.1276(50)[a]	76	0.29E-2
8	3	4474.0193	4474.0161(30)	-31	0.56E-2	8	3	4456.8268	4456.8245(30)	-22	0.59E-2
8	4	4474.3826	4474.3814(30)	-10	0.29E-2	8	4	4456.4385	4456.2643(30)[a]	-1741	0.30E-2
8	5	4474.9269	4474.9274(100)	6	0.29E-2	8	5	4455.9480	4456.1158(30)[a]	1678	0.30E-2
8	6	4475.7029	4475.6779(30)[a]	-249	0.57E-2	8	6	4455.3761	4455.3112(30)[a]	-649	0.59E-2
8	7	4476.8022	4476.1197(50)[a]	-6824	0.26E-2	8	7	4454.7147	4454.3033(30)[a]	-4113	0.27E-2
8	8	4478.3961	4478.3971(30)	10	0.18E-2	8	8	4453.8821	4453.2799(500)[a]	-6021	0.19E-2
9	0	4490.4487	4490.1528(20)[a]	-2957	0.25E-2						
9	1	4490.4635	4490.5171(100)[a]	536	0.13E-2						
9	2	4490.5180	4490.5987(30)[a]	807	0.13E-2						
9	3	4490.6142	4490.7298(30)[a]	1156	0.27E-2						
9	4	4490.8264	4490.9224(20)[a]	960	0.14E-2						
9	5	4491.1615	4491.2471(30)[a]	855	0.15E-2						
9	6	4491.6856	4491.6891(30)[a]	35	0.31E-2						
9	7	4492.4873	4493.2591(30)[a]	7718	0.15E-2						
9	8	4493.7293	4494.5625(50)[a]	8332	0.14E-2						
9	9	4495.7241	4495.5530(50)[a]	-1711	0.20E-2						

then, that for $J \geq 5$, we find a rather poor correspondence between our wavenumbers and the preceding transition wavenumbers (*1*). The calculated intensities, which are also given in Tables I–IV, were found to be very helpful in the assignment procedure and, despite the approximation in the intensity calculation (see Section III), the agreement with the observed intensities is relatively good.

As remarked in Section III, a more detailed analysis of the wavenumbers and intensities of the transitions pertaining to the $\nu_1 + \nu_2$ state would require a simultaneous

TABLE IV

Transition Wavenumbers (cm^{-1}) and Intensities (cm^{-2} atm^{-1}) of the $\nu_1 + \nu_2 - \nu_2$ Band of $^{15}NH_3$

			sP(J,K)						aP(J,K)		
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
1	0	3363.7541	3363.7578(30)	37	0.20E-1	1	0	(3305.3906)	-------	----	0.0
2	0	(3343.0455)	-------	----	0.0	2	0	3285.6294	3285.6284(20)	-8	0.27E-1
2	1	3343.3861	3343.3855(50)	-5	0.12E-1	2	1	3285.5563	3285.5557(20)	-5	0.10E-1
3	0	3321.7619	3321.7671(500)	52	0.36E-1	3	0	(3265.8574)	-------	----	0.0
3	1	3322.0921	3322.0913(30)	-7	0.16E-1	3	1	3265.7846	3265.7872(30)	26	0.14E-1
3	2	3323.0932	3323.0918(50)	-14	0.11E-1	3	2	3265.5603	3265.5638(30)	35	0.89E-2
4	0	(3299.9564)	-------	----	0.0	4	0	3246.0807	3246.0801(20)	-4	0.27E-1
4	1	3300.2736	3300.2774(50)	37	0.15E-1	4	1	3246.0094	3246.0076(20)	-17	0.13E-1
4	2	3301.2347	3301.2332(50)	-14	0.13E-1	4	2	3245.7899	3245.7896(20)	-2	0.11E-1
4	3	3302.8736	3302.8706(500)	-29	0.17E-1	4	3	3245.4044	3245.4039(20)	-4	0.14E-1
5	0	3277.6938	3277.6919(500)	-17	0.25E-1	5	0	(3226.3024)	-------	----	0.0
5	1	3277.9957	3277.9937(50)	-20	0.12E-1	5	1	3226.2335	3226.2335(20)	0	0.10E-1
5	2	3278.9085	3278.9104(30)	19	0.11E-1	5	2	3226.0215	3226.0271(500)	56	0.95E-2
5	3	3280.4669	3280.4641(20)	-26	0.19E-1	5	3	3225.6518	3225.6522(20)	4	0.16E-1
5	4	3282.7270	3282.7278(30)	8	0.59E-2	5	4	3225.0899	3225.0877(30)	-20	0.50E-2
6	0	(3255.0509)	-------	----	0.0	6	0	3206.5254	3206.5265(20)	11	0.14E-1
6	1	3255.3354	3255.3358(50)	3	0.82E-2	6	1	3206.4593	3206.4593(30)	1	0.71E-2
6	2	3256.1918	3256.1907(20)	-10	0.79E-2	6	2	3206.2563	-------	----	0.68E-2
6	3	3257.6565	3257.6551(50)	-13	0.15E-1	6	3	3205.9014	3205.9005(50)	-8	0.12E-1
6	4	3259.7842	3259.7847(30)	5	0.61E-2	6	4	3205.3703	3205.3655(500)	-47	0.52E-2
6	5	3262.6571	3262.6463(50)[a]	-107	0.40E-2	6	5	3204.6176	3204.6207(50)	31	0.33E-2
7	0	3232.1195	3232.1265(500)	70	0.98E-2	7	0	(3186.7565)	-------	----	0.0
7	1	3232.3843	3232.3927(500)	84	0.49E-2	7	1	3186.6929	3186.6967(50)	38	0.43E-2
7	2	3233.1754	3233.1751(50)	-1	0.48E-2	7	2	3186.4984	3186.4955(500)	-28	0.42E-2
7	3	3234.5302	3234.5332(500)	30	0.94E-2	7	3	3186.1679	3186.1819(500)	140	0.81E-2
7	4	3236.5071	3236.5062(50)	-8	0.44E-2	7	4	3185.6598	3185.6627(50)	29	0.37E-2
7	5	3239.1828	3239.1834(50)	7	0.37E-2	7	5	3184.9579	3184.9584(50)	5	0.32E-2
7	6	3242.6742	3242.6541(30)[a]	-200	0.49E-2	7	6	3183.9939	3183.9916(50)	-22	0.41E-2
8	0	(3209.0125)	-------	----	0.0	8	0	3167.0114	3167.0121(50)	7	0.46E-2
8	1	3209.2549	3209.2594(50)	45	0.26E-2	8	1	3166.9491	-------	----	0.23E-2
8	2	3209.9705	3209.9694(500)	-11	0.26E-2	8	2	3166.7602	3166.7604(50)	3	0.23E-2
8	3	3211.2032	3211.2045(50)	12	0.52E-2	8	3	3166.4337	3166.4365(500)	27	0.46E-2
8	4	3213.0019	-------	----	0.26E-2	8	4	3165.9620	-------	----	0.22E-2
8	5	3215.4509	3215.4466(50)[a]	-42	0.25E-2	8	5	3165.3086	-------	----	0.21E-2
8	6	3218.6607	-------	----	0.43E-2	8	6	3164.4337	3164.4467(500)[a]	131	0.36E-2
8	7	3222.8037	-------	----	0.14E-2	8	7	3163.2383	3163.2116(50)[a]	-266	0.12E-2
9	0	3185.8767	3185.8752(100)	-14	0.25E-2	9	0	(3147.3212)	-------	----	0.0
9	1	3186.0939	-------	----	0.12E-2	9	1	3147.2579	-------	----	0.11E-2
9	2	3186.7213	-------	----	0.13E-2	9	2	3147.0681	-------	----	0.11E-2
9	3	3187.8011	3187.8103(100)	92	0.26E-2	9	3	3146.7690	-------	----	0.23E-2
9	4	3189.4035	3189.4018(100)	-17	0.13E-2	9	4	3146.2917	-------	----	0.11E-2
9	5	3191.5898	-------	----	0.13E-2	9	5	3145.6759	-------	----	0.11E-2
9	6	3194.4736	-------	----	0.26E-2	9	6	3144.8828	-------	----	0.22E-2
9	7	3198.2199	-------	----	0.11E-2	9	7	3143.8461	-------	----	0.97E-3
9	8	3203.0985	-------	----	0.79E-3	9	8	3142.4003	-------	----	0.66E-3
10	0	(3162.9149)	-------	----	0.0	10	0	3127.7408	-------	----	0.95E-3
10	1	3163.1033	-------	----	0.53E-3	10	1	3127.6724	-------	----	0.48E-3
10	2	3163.6257	-------	----	0.54E-3	10	2	3127.4710	-------	----	0.49E-3
10	3	3164.5466	3164.5481(30)	15	0.11E-2	10	3	3127.1317	-------	----	0.10E-2
10	4	3165.8953	3165.8942(30)	-10	0.58E-3	10	4	3126.6821	-------	----	0.52E-3
10	5	3167.7720	-------	----	0.61E-3	10	5	3126.0820	-------	----	0.53E-3
10	6	3170.2726	-------	----	0.13E-2	10	6	3125.3502	-------	----	0.11E-2
10	7	3173.5540	-------	----	0.63E-3	10	7	3124.4588	-------	----	0.54E-3
10	8	3177.8717	-------	----	0.57E-3	10	8	3123.2994	-------	----	0.49E-3
10	9	3183.6620	-------	----	0.82E-3	10	9	3121.5858	-------	----	0.68E-3
11	0	3140.4192	-------	----	0.41E-3						
11	1	3140.5744	-------	----	0.21E-3						
11	2	3140.9688	-------	----	0.21E-3						
11	3	3141.6549	-------	----	0.44E-3						
11	4	3142.7404	-------	----	0.23E-3						
11	5	3144.2447	-------	----	0.25E-3						
11	6	3146.2855	-------	----	0.53E-3						
11	7	3149.0109	-------	----	0.28E-3						
11	8	3152.6612	-------	----	0.29E-3						
11	9	3157.6479	-------	----	0.54E-3						
11	10	3164.6822	-------	----	0.20E-3						

[a] Lines not used in the least squares fit in obtaining molecular parameters.

TABLE IV—*Continued*

sQ(J,K)						aQ(J,K)					
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
0	0	(3383.8474)	-------	----	0.0	0	0	(3325.1300)	-------	----	0.0
1	0	(3383.2048)	-------	----	0.0	1	0	(3325.0914)	-------	----	0.0
1	1	3383.5551	3383.5541(500)	-9	0.15E-1	1	1	3325.0233	3325.0254(30)	21	0.12E-1
2	0	(3381.9333)	-------	----	0.0	2	0	(3325.0082)	-------	----	0.0
2	1	3382.2777	3382.2797(100)	20	0.69E-2	2	1	3324.9430	3324.9416(30)	-12	0.57E-2
2	2	3383.3225	3383.3195(30)	-29	0.29E-1	2	2	3324.7412	3324.7405(30)	-6	0.24E-1
3	0	(3380.0598)	-------	----	0.0	3	0	(3324.8696)	-------	----	0.0
3	1	3380.3957	3380.4074(500)	117	0.36E-2	3	1	3324.8084	3324.8020(500)	-63	0.30E-2
3	2	3381.4140	3381.4135(50)	-4	0.15E-1	3	2	3324.6190	3324.6352(500)	162	0.13E-1
3	3	3383.1494	3383.1518(30)	24	0.75E-1	3	3	3324.2838	3324.2827(500)	-10	0.62E-1
4	0	(3377.6244)	-------	----	0.0	4	0	(3324.6615)	-------	----	0.0
4	1	3377.9490	-------	----	0.19E-2	4	1	3324.6052	3324.6058(50)	6	0.16E-2
4	2	3378.9322	-------	----	0.80E-2	4	2	3324.4310	3324.4280(30)	-29	0.67E-2
4	3	3380.6091	3380.6088(20)	-2	0.39E-1	4	3	3324.1223	3324.1201(50)	-21	0.33E-1
4	4	3383.0377	3383.0400(50)	23	0.40E-1	4	4	3323.6497	3323.6506(30)	9	0.33E-1
5	0	(3374.6807)	-------	----	0.0	5	0	(3324.3698)	-------	----	0.0
5	1	3374.9914	-------	----	0.95E-3	5	1	3324.3188	-------	----	0.81E-3
5	2	3375.9305	3375.9306(30)	1	0.40E-2	5	2	3324.1613	3324.1535(500)	-76	0.34E-2
5	3	3377.5340	3377.5348(50)	8	0.20E-1	5	3	3323.8838	3323.8796(50)	-41	0.17E-1
5	4	3379.8601	3379.8598(50)	-2	0.20E-1	5	4	3323.4560	3323.4607(50)	47	0.17E-1
5	5	3382.9927	3383.0009(500)[a]	82	0.37E-1	5	5	3322.8390	3322.8401(100)	11	0.30E-1
6	0	(3371.2990)	-------	----	0.0	6	0	(3323.9840)	-------	----	0.0
6	1	3371.5930	-------	----	0.45E-3	6	1	3323.9381	3323.9411(500)	30	0.39E-3
6	2	3372.4783	3372.4821(30)	38	0.19E-2	6	2	3323.7969	-------	----	0.16E-2
6	3	3373.9925	3373.9911(50)	-13	0.94E-2	6	3	3323.5478	3323.5500(100)	22	0.80E-2
6	4	3376.1936	3376.1877(30)	-58	0.94E-2	6	4	3323.1692	-------	----	0.80E-2
6	5	3379.1648	3379.1667(30)	19	0.17E-1	6	5	3322.6259	-------	----	0.14E-1
6	6	3383.0269	3383.0012(500)	-256	0.61E-1	6	6	3321.8554	3321.8564(50)	10	0.50E-1
7	0	(3367.5728)	-------	----	0.0	7	0	(3323.5030)	-------	----	0.0
7	1	3367.8471	-------	----	0.20E-3	7	1	3323.4610	-------	----	0.17E-3
7	2	3368.6677	-------	----	0.84E-3	7	2	3323.3333	-------	----	0.73E-3
7	3	3370.0739	3370.0734(500)	-4	0.41E-2	7	3	3323.1152	-------	----	0.36E-2
7	4	3372.1248	3372.1244(100)	-2	0.42E-2	7	4	3322.7757	-------	----	0.36E-2
7	5	3374.9017	3374.9023(20)	5	0.76E-2	7	5	3322.3039	3322.3037(50)	-1	0.64E-2
7	6	3378.5228	3378.5241(30)	13	0.27E-1	7	6	3321.6507	3321.6609(30)[a]	102	0.22E-1
7	7	3383.1671	3383.0745(500)[a]	-925	0.23E-1	7	7	3320.7167	3320.6829(50)[a]	-338	0.19E-1
8	0	(3363.6322)	-------	----	0.0	8	0	(3322.9411)	-------	----	0.0
8	1	3363.8833	-------	----	0.82E-4	8	1	3322.9006	-------	----	0.72E-4
8	2	3364.6256	-------	----	0.34E-3	8	2	3322.7803	-------	----	0.30E-3
8	3	3365.9016	-------	----	0.17E-2	8	3	3322.5748	-------	----	0.15E-2
8	4	3367.7712	-------	----	0.17E-2	8	4	3322.2734	-------	----	0.15E-2
8	5	3370.3143	3370.3137(500)[a]	-6	0.31E-2	8	5	3321.8621	-------	----	0.27E-2
8	6	3373.6457	3373.6447(100)	-9	0.11E-1	8	6	3321.3187	3321.5937(20)[a]	2751	0.92E-2
8	7	3377.9376	3377.9372(100)	-3	0.93E-2	8	7	3320.5768	3320.5151(30)[a]	-616	0.78E-2
8	8	3383.4686	3383.2636(20)[a]	-2050	0.16E-1	8	8	3319.4705	3319.4700(20)	-4	0.13E-1
9	0	(3359.6655)	-------	----	0.0	9	0	(3322.3370)	-------	----	0.0
9	1	3359.8888	-------	----	0.31E-4	9	1	3322.2940	-------	----	0.28E-4
9	2	3360.5354	-------	----	0.13E-3	9	2	3322.1706	-------	----	0.12E-3
9	3	3361.6524	-------	----	0.64E-3	9	3	3321.9786	-------	----	0.57E-3
9	4	3363.3014	-------	----	0.64E-3	9	4	3321.6791	-------	----	0.56E-3
9	5	3365.5603	-------	----	0.12E-2	9	5	3321.3058	-------	----	0.10E-2
9	6	3368.5401	-------	----	0.41E-2	9	6	3320.8514	3320.7947(50)[a]	-566	0.35E-2
9	7	3372.4055	3371.7277(100)[a]	-6777	0.35E-2	9	7	3320.2879	-------	----	0.30E-2
9	8	3377.4217	3377.4230(30)	13	0.60E-2	9	8	3319.5066	-------	----	0.50E-2
9	9	3384.0368	3383.5373(100)[a]	-4995	0.21E-1	9	9	3318.2205	3317.5195(20)[a]	-7008	0.17E-1
10	0	(3355.9527)	-------	----	0.0						
10	1	3356.1423	-------	----	0.11E-4						
10	2	3356.6704	-------	----	0.46E-4						
10	3	3357.5893	-------	----	0.22E-3						
10	4	3358.9665	-------	----	0.22E-3						
10	5	3360.8744	-------	----	0.41E-3						
10	6	3363.4212	-------	----	0.14E-2						
10	7	3366.7633	-------	----	0.12E-2						
10	8	3371.1511	-------	----	0.21E-2						
10	9	3377.0086	3376.8361(20)[a]	-1724	0.71E-2						
10	10	3385.0619	-------	----	0.62E-2						

TABLE IV—*Continued*

sR(J,K)						aR(J,K)					
J	K	CALC	EXP	DIF	INT	J	K	CALC	EXP	DIF	INT
0	0	(3403.2981)	-------	----	0.0	0	0	3344.8308	3344.8332(30)	24	0.18E-1
1	0	3422.0926	3422.0907(100)	-18	0.40E-1	1	0	(3364.4702)	-------	----	0.0
1	1	3422.4468	3422.4427(500)	-39	0.15E-1	1	1	3364.4100	3364.4116(20)	16	0.13E-1
2	0	(3440.2313)	-------	----	0.0	2	0	3384.0204	3384.0180(30)	-23	0.41E-1
2	1	3440.5813	3440.5792(30)	-20	0.22E-1	2	1	3383.9667	3383.9677(20)	10	0.19E-1
2	2	3441.6432	3441.6466(30)	33	0.15E-1	2	2	3383.7999	3383.8000(20)	1	0.12E-1
3	0	3457.7279	3457.7264(30)	-14	0.50E-1	3	0	(3403.4504)	-------	----	0.0
3	1	3458.0710	3458.0728(30)	18	0.24E-1	3	1	3403.4041	3403.4008(500)	-33	0.20E-1
3	2	3459.1115	3459.1124(20)	9	0.20E-1	3	2	3403.2601	3403.2611(20)	11	0.17E-1
3	3	3460.8849	3460.8841(30)	-8	0.26E-1	3	3	3403.0018	3402.9942(500)	-74	0.21E-1
4	0	(3474.6114)	-------	----	0.0	4	0	3422.7289	3422.7279(500)	-9	0.36E-1
4	1	3474.9446	3474.9461(30)	15	0.21E-1	4	1	3422.6905	3422.6945(50)	40	0.18E-1
4	2	3475.9541	3475.9578(30)	37	0.19E-1	4	2	3422.5707	3422.5714(50)	7	0.16E-1
4	3	3477.6763	3477.6792(30)	29	0.32E-1	4	3	3422.3543	3422.3487(50)	-56	0.27E-1
4	4	3480.1708	3480.1719(50)	12	0.10E-1	4	4	3422.0158	3422.0179(20)	21	0.84E-2
5	0	3490.9288	3490.9309(20)	21	0.32E-1	5	0	(3441.8284)	-------	----	0.0
5	1	3491.2489	3491.2552(500)	63	0.16E-1	5	1	3441.7976	3441.7974(30)	-1	0.13E-1
5	2	3492.2170	3492.2163(30)	-6	0.15E-1	5	2	3441.7019	3441.7025(30)	6	0.13E-1
5	3	3493.8701	3493.8709(30)	8	0.28E-1	5	3	3441.5302	3441.5291(30)	-10	0.24E-1
5	4	3496.2694	3496.2686(20)	-8	0.12E-1	5	4	3441.2549	3441.2555(20)	5	0.98E-2
5	5	3499.5004	3499.4934(500)	-69	0.76E-2	5	5	3440.8473	3440.8473(20)	0	0.63E-2
6	0	(3506.7523)	-------	----	0.0	6	0	3460.7305	3460.7332(50)	27	0.18E-1
6	1	3507.0558	3507.0554(20)	-3	0.10E-1	6	1	3460.7062	3460.7054(50)	-7	0.89E-2
6	2	3507.9707	-------	----	0.10E-1	6	2	3460.6318	-------	----	0.88E-2
6	3	3509.5363	3509.5369(500)	6	0.20E-1	6	3	3460.4952	3460.5042(500)	90	0.17E-1
6	4	3511.8113	3511.8118(30)	5	0.93E-2	6	4	3460.2851	3460.2862(20)	11	0.79E-2
6	5	3514.8838	3514.8857(20)	20	0.80E-2	6	5	3459.9720	3459.9732(30)	12	0.67E-2
6	6	3518.8754	3518.8762(30)	8	0.11E-1	6	6	3459.5122	3459.5203(50)[a]	82	0.87E-2
7	0	3522.1926	3522.1904(30)	-21	0.12E-1	7	0	(3479.4327)	-------	----	0.0
7	1	3522.4755	3522.4704(100)	-50	0.61E-2	7	1	3479.4125	3479.4119(30)	-4	0.53E-2
7	2	3523.3227	3523.3220(50)	-6	0.62E-2	7	2	3479.3534	3479.3560(30)	26	0.53E-2
7	3	3524.7722	3524.7783(20)	61	0.12E-1	7	3	3479.2563	3479.2666(500)	103	0.11E-1
7	4	3526.8940	3526.8909(50)	-31	0.61E-2	7	4	3479.0870	3479.0989(30)[a]	119	0.52E-2
7	5	3529.7652	3529.7691(20)	39	0.58E-2	7	5	3478.8574	3478.8641(50)	66	0.49E-2
7	6	3533.5079	3533.5085(100)	7	0.10E-1	7	6	3478.5357	3478.8138(30)[a]	2781	0.85E-2
7	7	3538.3010	3538.2983(500)	-26	0.34E-2	7	7	3478.0553	3477.9866(30)[a]	-686	0.28E-2
8	0	(3537.4211)	-------	----	0.0	8	0	3497.9569	3497.9563(30)	-5	0.57E-2
8	1	3537.6781	3537.6833(100)	52	0.32E-2	8	1	3497.9367	-------	----	0.29E-2
8	2	3538.4397	3538.4436(100)	39	0.33E-2	8	2	3497.8828	-------	----	0.29E-2
8	3	3539.7528	3539.7514(20)	-12	0.67E-2	8	3	3497.7844	3497.7832(500)[a]	-10	0.58E-2
8	4	3541.6690	3541.6740(30)	50	0.34E-2	8	4	3497.6608	3497.4868(50)[a]	-1738	0.30E-2
8	5	3544.2848	3544.2841(20)	-5	0.34E-2	8	5	3497.4920	3497.6546(50)[a]	1626	0.30E-2
8	6	3547.7122	3547.6880(20)[a]	-241	0.67E-2	8	6	3497.2873	-------	----	0.57E-2
8	7	3552.1231	3551.4492(50)[a]	-6739	0.30E-2	8	7	3497.0187	3496.6255(30)[a]	-3930	0.25E-2
8	8	3557.7919	-------	----	0.21E-2	8	8	3496.5767	-------	----	0.17E-2
9	0	3552.7033	3552.4104(30)[a]	-2929	0.31E-2						
9	1	3552.9277	-------	----	0.15E-2						
9	2	3553.5801	3553.6623(100)[a]	822	0.16E-2						
9	3	3554.6951	3554.8081(30)[a]	1129	0.32E-2						
9	4	3556.3726	3556.4680(50)[a]	954	0.17E-2						
9	5	3558.6627	3558.7482(30)[a]	856	0.18E-2						
9	6	3561.6886	3561.6938(20)[a]	52	0.37E-2						
9	7	3565.6148	3566.3830(100)[a]	7682	0.18E-2						
9	8	3570.7011	3571.5361(100)[a]	8350	0.17E-2						
9	9	3577.3835	3577.2145(30)[a]	-1689	0.24E-2						

analysis of all vibrational states that perturb the $\nu_1 + \nu_2$ state, especially the $\nu_2 + 2\nu_4$ and $\nu_2 + \nu_3$ vibrational states. Nevertheless, the results presented in this paper can be immediately used in astrophysical studies of planetary atmospheres, e.g., for obtaining reasonable information on the $^{14}NH_3/^{15}NH_3$ ratio. Finally, the molecular parameters of the $\nu_1 + \nu_2$ states of $^{14}NH_3$ and $^{15}NH_3$ offer important data on the mixing of the $|v_1\rangle$ and $|v_2\rangle$ vibrational wavefunctions and can be used to refine the potential function of NH_3 (7).

TABLE V

Parameters of the $\nu_1 + \nu_2$ States of $^{14}NH_3$ and $^{15}NH_3$ (in cm^{-1})

Parameter	$^{14}NH_3$	$^{15}NH_3$	Parameter	$^{14}NH_3$	$^{15}NH_3$
$^{(s)}E_0$	4294.50927(73)	4288.02448(62)	ΔE_0	25.5205(10)	24.27952(88)
$^{(s)}B$	9.87772(12)	9.85231(11)	ΔB	-0.12916(17)	-0.12584(15)
$^{(s)}C-^{(s)}B$	-3.80901(28)	-3.78035(23)	$\Delta(C-B)$	0.17907(37)	0.17391(31)
$^{(s)}D_J$	$0.9210(62) \times 10^{-3}$	$0.9585(55) \times 10^{-3}$	ΔD_J	$-4.090(87) \times 10^{-4}$	$-3.950(77) \times 10^{-4}$
$^{(s)}D_{JK}$	$-2.052(25) \times 10^{-3}$	$-1.989(20) \times 10^{-3}$	ΔD_{JK}	$11.00(30) \times 10^{-4}$	$10.26(25) \times 10^{-4}$
$^{(s)}D_K$	$1.301(22) \times 10^{-3}$	$1.241(21) \times 10^{-3}$	ΔD_K	$-7.03(27) \times 10^{-4}$	$-6.59(26) \times 10^{-4}$
$^{(s)}H_{JJJ}$	$0.81(11) \times 10^{-6}$	$1.19(10) \times 10^{-6}$	ΔH_{JJJ}	$-1.44(15) \times 10^{-6}$	$-1.34(14) \times 10^{-6}$
$^{(s)}H_{JJK}$	$-7.57(64) \times 10^{-6}$	$-3.36(51) \times 10^{-6}$	ΔH_{JJK}	$4.80(74) \times 10^{-6}$	$2.09(61) \times 10^{-6}$
$^{(s)}H_{JKK}$	$5.05(129) \times 10^{-6}$	$2.44(108) \times 10^{-6}$	ΔH_{JKK}	$0.61(140) \times 10^{-6}$	$1.39(133) \times 10^{-6}$
$^{(s)}H_{KKK}$	$0.543(952) \times 10^{-6}$	$-0.899(798) \times 10^{-6}$	ΔH_{KKK}	$-2.88(102) \times 10^{-6}$	$-1.18(102) \times 10^{-6}$
$^{(s)}G_{JJJJ}$	$0.414(62) \times 10^{-8}$	$0.111(59) \times 10^{-8}$	ΔG_{JJJJ}	$1.067(87) \times 10^{-8}$	$0.942(81) \times 10^{-8}$
$^{(s)}G_{JJJK}$	$2.51(48) \times 10^{-8}$	$-1.27(36) \times 10^{-8}$	ΔG_{JJJK}	$-3.14(54) \times 10^{-8}$	$-0.90(45) \times 10^{-8}$
$^{(s)}G_{JJKK}$	$3.36(105) \times 10^{-8}$	$1.77(78) \times 10^{-8}$	ΔG_{JJKK}	$-8.46(117) \times 10^{-8}$	$-1.84(116) \times 10^{-8}$
$^{(s)}G_{JKKK}$	$-0.44(321) \times 10^{-8}$	$6.91(210) \times 10^{-8}$	ΔG_{JKKK}	$8.22(325) \times 10^{-8}$	$-9.42(233) \times 10^{-8}$
$^{(s)}G_{KKKK}$	$-5.25(297) \times 10^{-8}$	$-6.37(203) \times 10^{-8}$	ΔG_{KKKK}	$1.68(299) \times 10^{-8}$	$11.4(22) \times 10^{-8}$
η	$-1.72(27) \times 10^{-8}$	$-0.81(18) \times 10^{-8}$	α	$-0.676(330) \times 10^{-4}$	$-0.75(16) \times 10^{-4}$

ACKNOWLEDGMENTS

The authors thank V. Špirko and D. Papoušek for reading the manuscript and suggesting improvements.

RECEIVED: May 27, 1985

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