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A Simultaneous Analysis of the Microwave, Submillimeterwave, and Infrared Transitions between the Ground and ν_2 Inversion–Rotation Levels of $^{15}NH_3$

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The submillimeterwave spectra of the pure inversion and inversion–rotation transitions in the ν_2 excited state (79 transitons) and the diode laser spectra of the ν_2 band (83 transitions) of $^{15}NH_3$ have been measured. A simultaneous least squares analysis has been carried out of these data together with previously published wavenumbers of the pure inversion transitions and inversion–rotation transitions in the ground state measured by the microwave and Fourier spectroscopy, and the ν_2 band transition frequencies obtained by the infrared-microwave two-photon technique. A theory of the $\Delta k = \pm 3n$ interactions in the ground and ν_2 excited states of ammonia (Š. Urban, V. Špirko, D. Papoušek, J. Kauppinen, S. P. Belov, L. I. Gershtein, and A. F. Krupnov, *J. Mol. Spectrosc.* **88**, 274–282 (1981)) has been used in the analysis. The "smoothed" values of the ν_2 band wavenumbers can be used for calibration purposes with better than 1×10^{-3} cm^{-1} precision.

I. INTRODUCTION

In two previous papers (*1, 2*), we have described a simultaneous analysis of the microwave, submillimeterwave, Fourier transform infrared, standard diode laser, diode laser heterodyne, and infrared-microwave two-photon measurements of the transition frequencies between the ground and ν_2 inversion–rotation energy levels of $^{14}NH_3$. One of the main results of this work was to establish a calibration standard for the 10-μm region (ν_2 band of $^{14}NH_3$) with a precision better than 1×10^{-4} cm^{-1} (2).

An extension of this work to $^{15}NH_3$ is of importance for theory as well as applied spectroscopy. For example, precise experimental data on the transition frequencies of different isotopomers of the same molecule are important for the determination of a complete anharmonic potential function of the molecule (*3*). Furthermore, high and very high resolution infrared spectroscopy, especially diode laser spectroscopy, needs calibration standards of precision compatible with the resolution of the individual experimental techniques.

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As for the precise transition frequencies for $^{15}NH_3$ which could be used in a simultaneous analysis completely analogous to that described previously for $^{14}NH_3$ (*1, 4*), there are excellent microwave data on the ground state pure inversion transitions (*5*) of $^{15}NH_3$ up to $J = 10$ and a precise ground state inversion–rotation transition frequency $J = 1 \leftarrow 0$, $K = 0$ measured in the submillimeterwave region (*6*). The ground state inversion–rotation transition wavenumbers have been measured in the far-infrared region with a Fourier transform spectrometer (*7*). Although the resolution was about 0.03 cm^{-1}, these data are useful for determination of the ground state centrifugal distortion constants of $^{15}NH_3$ because they extend up to $J = 13$.

The ν_2 band transition frequencies of $^{15}NH_3$ measured with a precision better than 1×10^{-3} cm^{-1} are the infrared-microwave two-photon data (*8–10*), the few laser Stark data indicated in Ref. (*11*), and the highly precise data obtained by the diode laser heterodyne technique (*12, 13*).

We have extended these data by measuring 83 ν_2 band transition wavenumbers of $^{15}NH_3$ with a diode laser spectrometer, using $^{14}NH_3$ ν_2 band wavenumbers (*2*) as a calibration standard.

Furthermore, we have measured for the first time 76 pure inversion transition frequencies in the ν_2 state of $^{15}NH_3$ and 3 inversion–rotation transition frequencies. These transitions appear in the submillimeterwave region; we have also involved into our fit the previously published (*14*) millimeterwave transition frequency $J = 2 \leftarrow 1$, $K = 1$ and the submillimeterwave transition frequency (*15*) $J = 1 \leftarrow 0$, $K = 0$.

II. EXPERIMENTAL DETAILS

The high-sensitivity submillimeterwave spectrometer RAD (*16, 17*) at the Institute for Applied Physics of the Academy of Sciences, USSR, in Gorkii has been used (cf. Fig. 1). Besides measurements carried out with the microwave accuracy (rms error about ± 0.00003 cm^{-1}), we measured transition frequencies in the ν_2 state of $^{14}NH_3$ with the accuracy of the standard high resolution infrared spectroscopy (rms error about ± 0.001 cm^{-1}) (Table I). In those measurements, the $^{15}NH_3$ spectrum was recorded simultaneously with the SO_2 spectrum, and the $^{15}NH_3$ frequencies have been determined by interpolating between the SO_2 frequencies. The pressure of the ammonia sample (75% $^{15}NH_3$) in the acoustic cell was about 130 Pa (1 Torr); the experimental uncertainties of the measured frequencies are given in Table I.

The diode laser spectra with the Doppler limited resolution have been measured with a spectrometer described in Refs. (*18, 19*). The ammonia sample containing 95% $^{15}NH_3$ has been measured in a 1-m cell at the pressure $P \leq 65$ Pa (0.5 Torr). The $^{15}NH_3$ lines have been calibrated by means of the $^{14}NH_3$ ν_2 band wavenumbers (*2*). The $^{14}NH_3$ lines have been recorded with sufficient intensity either directly (cf. Fig. 2) or by measuring the $^{15}NH_3$ spectra simultaneously with the 0.6-m cell containing 0.3 Torr of pure $^{14}NH_3$ (Table II).

III. RESULTS AND DISCUSSION

A simultaneous least squares analysis of all the $^{15}NH_3$ transition frequencies mentioned in this paper has been done as described in detail in our previous papers (*1, 2, 4*). This means that the only vibrational–rotational interaction which has been

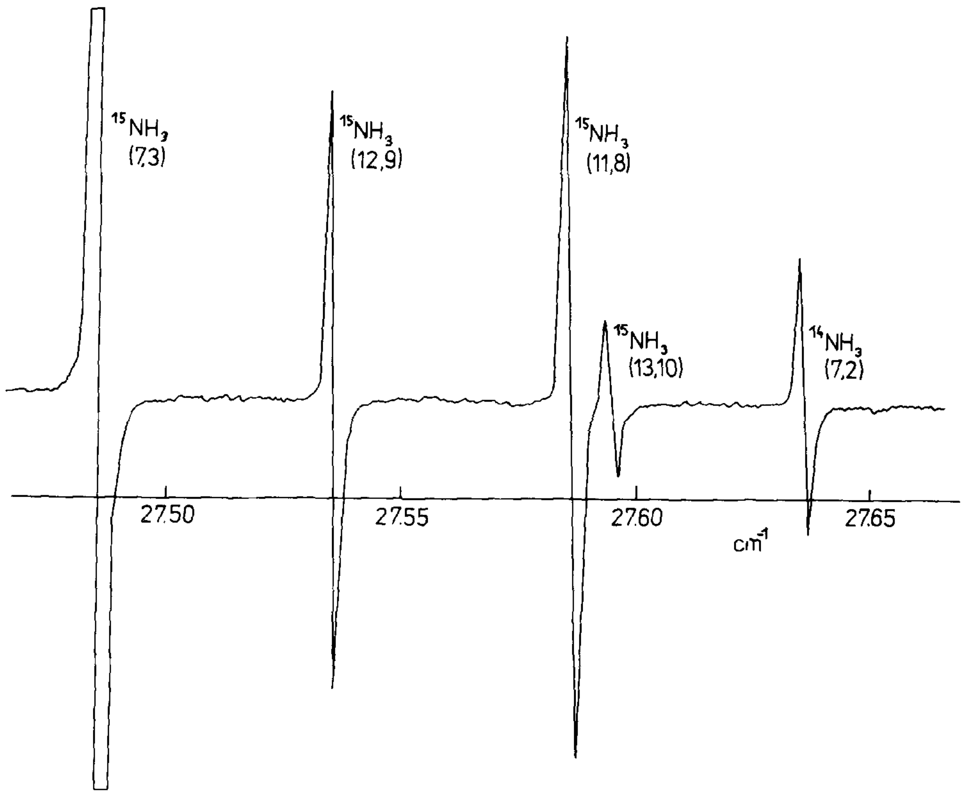

FIG. 1. Part of the submillimeterwave spectrum of $^{15}NH_3$.

considered explicitly was the $\Delta k = \pm 3n$ interaction; all other vibrational-rotational interactions have been "absorbed" into the effective spectroscopic parameters including the octic centrifugal distortion constants (Table III).

The values of the transition wavenumbers calculated from the molecular parameters in Table III are compared with the experimental data in Tables I and II. In the last column of Tables I and II, the intensities of the corresponding lines are given which were calculated as described in Ref. (*1*).

It is obvious from Tables I and II that we arrived at a quantitative description of the experimental data. The "smoothed" values of the transition wavenumbers of the ν_2 band have a precision estimated to be better than 1×10^{-3} cm^{-1} for all $J' < 10$ in the *Q*-branch lines and for all $J' < 8$ in the *R* and *P* branches. It should be emphasized that the calculated values of the ν_2 band *P*- and *R*-branch transition wavenumbers in Table II represent basically a transfer of the experimental information on the ground state, ν_2 state, and *Q*-branch transition wavenumbers to the $\Delta J = \mp 1$ ν_2 band transitions. Therefore, the precision of the calculated *P* and *R* wavenumbers in Table II is determined by the extent of the experimental data available for the *aR* branch transitions and by the precision of the measured ground state inversion–rotation transition wavenumbers (*7*).

TABLE I

Pure Inversion and Inversion-Rotation Transition Wavenumbers (cm^{-1}) and Intensities ($cm^{-2}\ atm^{-1}$) of $^{15}NH_3$ in the ν_2 State[a]

a ← s: $\Delta J = 0$, $\Delta K = 0$

J	K	CALC	EXP	$\delta \times 10^5$	INT
0	0	(34.43779)	------	---	0.
1	0	(34.08395)	------	---	0.
1	1	34.32985	34.33108(100)	124	0.24E-02
2	0	(33.38667)	------	---	0.
2	1	33.62785	33.62793(100)	8	0.11E-02
2	2	34.36094	34.36096(3)	2	0.47E-02
3	0	(32.36610)	------	---	0.
3	1	32.60055	32.60022(100)	-32	0.53E-03
3	2	33.31259	33.31138(100)	-120	0.23E-02
3	3	34.53073	34.53058(3)	-14	0.12E-01
4	0	(31.05161)	------	---	0.
4	1	31.27751	31.27864(100)	113	0.26E-03
4	2	31.96234	31.96278(100)	44	0.11E-02
4	3	33.13430	33.13392(100)	-37	0.60E-02
4	4	34.84093	34.84077(100)	-15	0.66E-02
5	0	(29.48012)	------	---	0.
5	1	29.69605	29.69621(100)	16	0.12E-03
5	2	30.34824	30.34799(100)	-24	0.52E-03
5	3	31.46267	31.46210(100)	-56	0.27E-02
5	4	33.09008	33.09023(100)	14	0.30E-02
5	5	35.29324	35.29308(100)	-15	0.63E-02
6	0	(27.69473)	------	---	0.
6	1	27.89966	27.89863(100)	-101	0.49E-04
6	2	28.51460	28.51439(100)	-19	0.22E-03
6	3	29.56748	29.56679(100)	-69	0.11E-02
6	4	31.09998	31.09851(100)	-146	0.13E-02
6	5	33.17881	33.17762(100)	-118	0.26E-02
6	6	35.89141	------	---	0.11E-01
7	0	(25.74275)	------	---	0.
7	1	25.93613	25.93628(100)	15	0.19E-04
7	2	26.51012	26.51007(3)	-4	0.84E-04
7	3	27.48539	27.48535(100)	-4	0.44E-03
7	4	28.92292	28.92167(100)	-124	0.49E-03
7	5	30.86489	30.86402(100)	-87	0.10E-02
7	6	33.40012	33.39977(100)	-34	0.41E-02
7	7	36.64024	------	---	0.42E-02
8	0	(23.67383)	------	---	0.
8	1	23.85564	23.85569(3)	5	0.66E-05
8	2	24.38596	24.38654(100)	58	0.29E-04
8	3	25.29583	25.29650(100)	67	0.15E-03
8	4	26.61376	26.61374(100)	0	0.17E-03
8	5	28.40952	28.40932(100)	-19	0.35E-03
8	6	30.75512	30.75528(100)	16	0.14E-02
8	7	33.75497	33.75535(100)	38	0.15E-02
8	8	37.54586	------	---	0.31E-02
9	0	(21.53799)	------	---	0.
9	1	21.70865	21.70882(100)	17	0.21E-05
9	2	22.19372	22.19389(3)	17	0.52E-05
9	3	23.00148	23.00128(3)	-19	0.48E-04
9	4	24.22773	24.22709(100)	-62	0.54E-04
9	5	25.87117	25.87123(100)	6	0.11E-03
9	6	28.01907	28.01907(3)	0	0.45E-03
9	7	30.76620	30.76662(100)	42	0.47E-03
9	8	34.24551	34.24669(100)	119	0.97E-03
9	9	38.61573	------	---	0.42E-02

a ← s: $\Delta J = 0$, $\Delta K = 0$

J	K	CALC	EXP	$\delta \times 10^5$	INT
10	0	(19.38386)	------	---	0.
10	1	19.54528	19.54516(3)	-11	0.60E-06
10	2	19.98384	19.98383(3)	0	0.26E-05
10	3	20.74234	20.74247(3)	13	0.14E-04
10	4	21.81847	21.81976(100)	129	0.15E-04
10	5	23.30663	23.30612(100)	-50	0.32E-04
10	6	25.25286	25.25314(100)	28	0.13E-03
10	7	27.74605	27.74653(100)	46	0.13E-03
10	8	30.90286	30.90271(100)	-14	0.28E-03
10	9	34.87505	------	---	0.12E-02
10	10	39.85870	------	---	0.13E-02
11	0	(17.25730)	------	---	0.
11	1	17.41226	------	---	0.15E-06
11	2	17.80444	------	---	0.68E-06
11	3	18.41704	18.41717(3)	13	0.35E-05
11	4	19.43638	19.43615(3)	-22	0.39E-05
11	5	20.76916	20.76927(3)	11	0.62E-05
11	6	22.51358	22.51358(100)	0	0.33E-04
11	7	24.75049	24.75050(3)	1	0.34E-04
11	8	27.58612	27.58609(300)	196	0.71E-04
11	9	31.15890	31.15889(100)	0	0.31E-03
12	5	18.30724	18.30900(100)	176	0.19E-05
12	6	19.85298	19.85240(100)	-57	0.77E-05
12	7	21.83764	21.83744(100)	-19	0.78E-05
12	8	24.35699	24.35752(100)	53	0.16E-04
12	9	27.53605	27.53505(100)	-99	0.71E-04
12	10	31.53718	31.53615(100)	-102	0.79E-04
13	8	21.26925	21.26923(3)	-1	0.34E-05
13	9	24.06639	24.06632(100)	-6	0.15E-04
13	10	27.59357	27.59442(100)	85	0.16E-04
13	11	32.03959	32.03716(100)	-242	0.38E-04
14	8	18.36833	18.36637(300)	-194	0.64E-06
14	9	20.79999	20.80003(10)	5	0.27E-05
14	10	23.87368	23.87418(100)	50	0.31E-05
14	11	27.75731	27.75720(100)	-10	0.71E-05
16	11	20.12951	20.12926(100)	-24	0.18E-06
16	12	23.76553	23.76644(300)	91	0.87E-06
16	13	28.40158	28.40498(300)	340	0.11E-05

s ← a: $\Delta J = 1$, $\Delta K = 0$

J	K	CALC	EXP	$\delta \times 10^5$	INT
0	0	-14.34454	-14.34453(1)[b]	-1	0.22E-03
1	0	(6.07532)			0.
1	1	5.83913	5.83920(5)[c]	-7	0.53E-04
2	0	26.78475	26.78473(3)	-2	0.42E-02
2	1	26.55780	26.55783(3)	3	0.19E-02
2	2	25.86822	25.86820(3)	-2	0.12E-02

[a] Our submillimeterwave measurements unless stated otherwise; CALC and EXP are calculated and observed transition wavenumbers; δ = EXP-CALC, INT are calculated intensities. Values in parentheses of the experimental wavenumbers are estimated experimental uncertainties in units of the last digit quoted.

[b] Ref.(15). [c] Ref.(14).

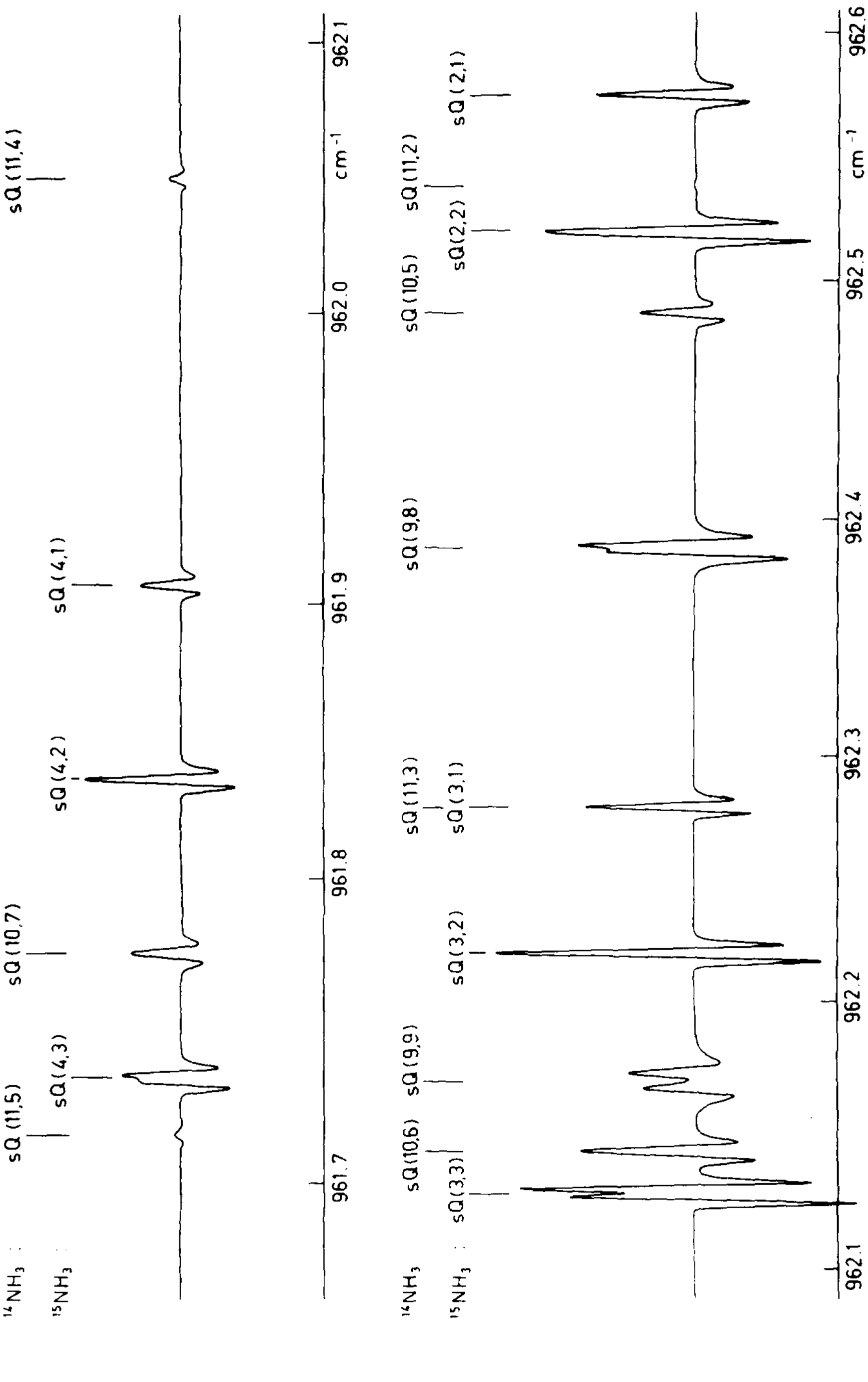

FIG. 2. The diode laser spectrum of the ν_2 band lines of $^{15}NH_3$ and $^{14}NH_3$.

TABLE II

Transition Wavenumbers (cm^{-1}) and Intensities (cm^{-2} atm^{-1}) in the ν_2 Band of $^{15}NH_3$[a]

		sP				
J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
1	0	943.05316	943.05370(100)	54	F DL	0.29E+01
2	0	(923.13035)	------	---		0.
2	1	923.10675	923.10640(20)	-24	C TC	0.18E+01
			923.10657(10)	-17	B LC	
3	0	903.14981	903.15009(40)	28	H DL	0.51E+01
3	1	903.12178	903.12165(60)	7	H DL	0.23E+01
3	2	903.03989	903.03979(60)	-9	H DL	0.15E+01
4	0	(883.13825)	------	---		0.
4	1	883.10528	------	---		0.21E+01
4	2	883.00842	------	---		0.18E+01
4	3	882.85386	------	---		0.23E+01
5	0	863.12470	------	---		0.34E+01
5	1	863.08636	------	---		0.16E+01
5	2	862.97325	------	---		0.15E+01
5	3	862.79112	------	---		0.25E+01
5	4	862.55082	------	---		0.81E+00
6	0	(843.13967)	------	---		0.
6	1	843.09567	------	---		0.11E+01
6	2	842.96541	------	---		0.11E+01
6	3	842.75280	------	---		0.19E+01
6	4	842.47123	------	---		0.82E+00
6	5	842.13207	------	---		0.53E+00
7	0	823.21424	------	---		0.13E+01
7	1	823.16441	------	---		0.64E+00
7	2	823.01657	------	---		0.63E+00
7	3	822.77434	------	---		0.12E+01
7	4	822.44800	------	---		0.57E+00
7	5	822.05003	------	---		0.49E+00
7	6	821.59982	------	---		0.64E+00
8	0	(803.37908)	------	---		0.
8	1	803.32341	------	---		0.33E+00
8	2	803.15804	------	---		0.33E+00
8	3	802.88145	------	---		0.66E+00
8	4	802.51397	------	---		0.33E+00
8	5	802.05656	------	---		0.31E+00
8	6	801.52911	------	---		0.54E+00
8	7	800.95634	------	---		0.18E+00
9	0	783.66359	------	---		0.30E+00
9	1	783.60220	------	---		0.35E+00
9	2	783.41994	------	---		0.15E+00
9	3	783.11508	------	---		0.31E+00
9	4	782.70061	------	---		0.16E+00
9	5	782.18447	------	---		0.16E+00
9	6	781.58054	------	---		0.32E+00
9	7	780.91028	------	---		0.14E+00
9	8	780.20423	------	---		0.99E-01
10	0	(764.09520)	------	---		0.

		sP				
J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
10	1	764.02835	------	---		0.63E-01
10	2	763.83046	------	---		0.64E-01
10	3	763.48731	------	---		0.13E+00
10	4	763.03712	------	---		0.69E-01
10	5	762.46418	------	---		0.73E-01
10	6	761.78617	------	---		0.15E+00
10	7	761.02129	------	---		0.75E-01
10	8	760.19561	------	---		0.69E-01
10	9	759.34646	------	---		0.99E-01
11	0	744.69904	------	---		0.47E-01
11	1	744.62706	------	---		0.24E-01
11	2	744.41567	------	---		0.24E-01
11	3	744.04804	------	---		0.51E-01
11	4	743.54990	------	---		0.27E-01
11	5	742.92298	------	---		0.29E-01
11	6	742.17463	------	---		0.61E-01
11	7	741.31988	------	---		0.33E-01
11	8	740.38038	------	---		0.34E-01
11	9	739.38749	------	---		0.64E-01
11	10	738.38642	------	---		0.24E-01
12	0	(725.49810)	------	---		0.
12	1	725.42136	------	---		0.80E-02
12	2	725.19990	------	---		0.83E-02
12	3	724.78655	------	---		0.17E-01
12	4	724.26250	------	---		0.93E-02
12	5	723.58492	------	---		0.10E-01
12	6	722.77078	------	---		0.22E-01
12	7	721.83220	------	---		0.12E-01
12	8	720.78663	------	---		0.13E-01
12	9	719.65963	------	---		0.28E-01
12	10	718.48862	------	---		0.14E-01
12	11	717.32805	------	---		0.11E-01
13	0	706.51403	------	---		0.49E-02
13	1	706.43287	------	---		0.25E-02
13	2	706.20759	------	---		0.25E-02
13	3	705.77110	------	---		0.54E-02
13	4	705.19613	------	---		0.29E-02
13	5	704.47115	------	---		0.32E-02
13	6	703.59594	------	---		0.70E-02
13	7	702.58011	------	---		0.40E-02
13	8	701.43729	------	---		0.45E-02
13	9	700.18763	------	---		0.10E-01
13	10	698.86111	------	---		0.55E-02
13	11	697.50213	------	---		0.56E-02
13	12	696.17586	------	---		0.68E-02

TABLE II—*Continued*

J	K	CALC	EXP (aQ)	$\delta \times 10^5$	ID[b]	INT
0	0	(962.89447)	------	---		0.
1	0	(962.79258)	------	---		0.
1	1	962.77528	------	---		0.22E+01
2	0	(962.59235)	------	---		0.
2	1	962.57373	962.57320(70)	-52	H DL	0.10E+01
2	2	962.52014	962.52038(30)	24	H DL	0.43E+01
3	0	(962.30067)	------	---		0.
3	1	962.28013	962.28014(60)	1	H DL	0.54E+00
			962.28034(20)	21	A LN	
3	2	962.22070	962.22065(70)	-4	H DL	0.23E+01
			962.22079(20)	9	A LN	
3	3	962.12887	962.12880(50)	-6	H DL	0.11E+02
			962.12828(100)	-58	A TN	
4	0	(961.92725)	------	---		0.
4	1	961.90429	961.90478(50)	49	H DL	0.28E+00
4	2	961.83748	961.83756(40)	8	H DL	0.12E+01
4	3	961.73311	961.73354(50)	43	H DL	0.58E+01
4	4	961.60229	961.60176(20)	-52	A LN	0.59E+01
5	0	(961.48400)	------	---		0.
5	1	961.45822	------	---		0.14E+00
5	2	961.38281	------	---		0.59E+00
5	3	961.26168	961.26199(50)	31	H DL	0.29E+01
5	4	961.11043	------	---		0.30E+01
5	5	960.94020	960.93999(60)	-20	H DL	0.54E+01
6	0	(960.98424)	------	---		0.
6	1	960.95536	------	---		0.66E-01
6	2	960.87055	------	---		0.28E+00
6	3	960.73520	------	---		0.14E+01
6	4	960.55685	960.55756(20)	71	C TC	0.14E+01
6	5	960.35297	960.35326(50)	29	H DL	0.26E+01
6	6	960.14345	960.14321(40)	-23	H DL	0.90E+01
7	0	(960.44184)	------	---		0.
7	1	960.40971	------	---		0.29E-01
7	2	960.31516	960.31512(60)	-3	H DL	0.12E+00
7	3	960.15451	960.15468(60)	17	H DL	0.61E+00
7	4	959.95737	959.95711(50)	-25	H DL	0.61E+00
7	5	959.71791	959.71795(40)	4	H DL	0.11E+01
			959.71764(20)	-26	C TC	
7	6	959.46071	959.46082(30)	11	H DL	0.39E+01
7	7	959.21299	959.21279(40)	-19	H DL	0.34E+01
			959.21256(20)	-42	C TC	
			959.21260(100)	-38	A TN	
8	0	(959.87048)	------	---		0.
8	1	959.83508	959.83465(50)	-42	H DL	0.12E-01
8	2	959.73097	959.73105(50)	8	H DL	0.50E-01
8	3	959.56270	959.56266(60)	-3	H DL	0.25E+00
8	4	959.32753	959.32813(80)	60	H DL	0.25E+00
8	5	959.05182	959.05171(50)	-10	H DL	0.46E+00
8	6	958.74594	958.74609(20)	15	C TC	0.16E+01
8	7	958.43406	------	---		0.14E+01
8	8	958.15007	958.14996(20)	-10	C TC	0.24E+01
			958.15001(20)	-5	L LS	
9	0	(959.28304)	------	---		0.
9	1	959.24445	959.24500(50)	55	H DL	0.45E-02
9	2	959.13160	959.13140(50)	-19	H DL	0.19E-01
9	3	958.92040	958.91999(50)	-40	H DL	0.93E-01
9	4	958.68184	958.68160(60)	-23	H DL	0.93E-01
9	5	958.37032	------	---		0.17E+00
9	6	958.01630	958.01593(20)	-36	C TC	0.60E+00
9	7	957.64085	957.64036(80)	-48	H DL	0.51E+00
9	8	957.27363	957.27421(80)	58	H DL	0.88E+00
9	9	956.95636	956.95674(50)	38	H DL	0.30E+01
10	0	(958.69124)	------	---		0.
10	1	958.64965	------	---		0.16E-02
10	2	958.52969	------	---		0.65E-02
10	3	958.33374	------	---		0.32E-01
10	4	958.03323	------	---		0.32E-01
10	5	957.68719	957.68709(20)	-9	C TC	0.59E-01
10	6	957.28682	957.28640(70)	-41	H DL	0.21E+00
10	7	956.85019	956.85030(20)	11	H DL	0.18E+00
10	8	956.40271	956.40269(20)	-1	C TC	0.30E+00
			956.40369(80)	98	H DL	
10	9	955.98036	955.98083(20)	47	E HD	0.10E+01
			955.98090(80)	54	H DL	
10	10	955.63394	------	---		0.50E+00
11	0	(958.10589)	------	---		0.
11	1	958.06151	------	---		0.49E-03
11	2	957.93739	------	---		0.21E-02
11	3	957.65624	------	---		0.10E-01
11	4	957.39304	------	---		0.10E-01
11	5	957.01427	957.01386(50)	-40	H DL	0.19E-01
11	6	956.57015	956.57040(20)	25	L LS	0.65E-01
11	7	956.07595	956.07600(50)	5	H DL	0.56E-01
			956.07567(60)	-27	H DL	
11	8	955.55304	955.54763(20)[c]	-540	C TC	0.95E-01
11	9	955.03178	955.03152(20)	-25	L LS	0.33E+00
11	10	954.55543	------	---		0.28E+00
11	11	954.18540	------	---		0.50E+00
12	0	(957.53763)	------	---		0.
12	1	957.49066	------	---		0.14E-03
12	2	957.36815	------	---		0.61E-03
12	3	957.15295	------	---		0.30E-02
12	4	956.77154	------	---		0.30E-02
12	5	956.36175	956.36177(50)	2	H DL	0.55E-02
12	6	955.87668	955.87773(100)	105	H DL	0.19E-01
12	7	955.32911	------	---		0.16E-01
12	8	954.73666	------	---		0.28E-01
12	9	954.12450	------	---		0.94E-01
12	10	953.52852	------	---		0.62E-01
12	11	953.00037	------	---		0.14E+00
12	12	952.61384	------	---		0.52E+00
13	0	(956.99860)	------	---		0.
13	1	956.94910	------	---		0.39E-04
13	2	956.84258	------	---		0.16E-03
13	3	956.43746	------	---		0.81E-03
13	4	956.17927	------	---		0.81E-03
13	5	955.73949	------	---		0.15E-02
13	6	955.21565	------	---		0.51E-02
13	7	954.61848	------	---		0.43E-02
13	8	953.96249	------	---		0.74E-02
13	9	953.26801	------	---		0.25E-01
13	10	952.56424	------	---		0.22E-01
13	11	951.89348	------	---		0.38E-01
13	12	951.31699	------	---		0.14E+00
13	13	950.92293	950.91534(20)[c]	-758	C TC	0.13E+00

TABLE II—*Continued*

J	K	CALC	sR EXP	$\delta\times10^5$	ID[b]	INT
0	0	(982.63388)	------	---		0.
1	0	1002.25457	------	---		0.61E+01
1	1	1002.24226	------	---		0.23E+01
2	0	(1021.74321)	------	---		0.
2	1	1021.73208	------	---		0.35E+01
2	2	1021.70095	------	---		0.23E+01
3	0	1041.08966	1041.08986(20)	20	E HD	0.79E+01
3	1	1041.07915	1041.07940(20)	25	E HD	0.37E+01
3	2	1041.04976	1041.04997(30)	21	E HD	0.32E+01
3	3	1041.00811	1041.00810(30)	0	E HD	0.40E+01
4	0	(1060.28655)	------	---		0.
4	1	1060.27616	------	---		0.33E+01
4	2	1060.24704	------	---		0.21E+01
4	3	1060.20367	------	---		0.51E+01
4	4	1060.16190	------	---		0.16E+01
5	0	1079.32856	------	---		0.51E+01
5	1	1079.31792	------	---		0.25E+01
5	2	1079.28795	------	---		0.24E+01
5	3	1079.24408	------	---		0.45E+01
5	4	1079.19605	------	---		0.19E+01
5	5	1079.16109	------	---		0.12E+01
6	0	(1098.21183)	------	---		0.
6	1	1098.20066	------	---		0.17E+01
6	2	1098.16914	------	---		0.17E+01
6	3	1098.11537	------	---		0.32E+01
6	4	1098.06622	------	---		0.15E+01
6	5	1098.02084	1098.02083(20)	0	L LS	0.13E+01
6	6	1098.00435	1098.00475(20)	40	L LS	0.17E+01
7	0	1116.93324	------	---		0.20E+01
7	1	1116.92138	------	---		0.10E+01
7	2	1116.88809	------	---		0.10E+01
7	3	1116.83576	------	---		0.20E+01
7	4	1116.77093	------	---		0.10E+01
7	5	1116.71317	------	---		0.95E+00
7	6	1116.67755	------	---		0.17E+01
7	7	1116.69071	------	---		0.57E+00
8	0	(1135.48993)	------	---		0.
8	1	1135.47733	------	---		0.53E+00
8	2	1135.44263	------	---		0.54E+00
8	3	1135.36802	------	---		0.11E+01
8	4	1135.30877	------	---		0.56E+00
8	5	1135.23766	------	---		0.57E+00
8	6	1135.18170	------	---		0.11E+01
8	7	1135.16463	------	---		0.50E+00
8	8	1135.21948	------	---		0.35E+00
9	0	1153.87906	------	---		0.50E+00
9	1	1153.86576	------	---		0.25E+00
9	2	1153.83082	------	---		0.26E+00
9	3	1153.76684	------	---		0.54E+00
9	4	1153.67796	------	---		0.28E+00
9	5	1153.59334	------	---		0.29E+00
9	6	1153.51695	------	---		0.61E+00
9	7	1153.46975	------	---		0.31E+00
9	8	1153.48073	------	---		0.28E+00
9	9	1153.59026	------	---		0.41E+00

J	K	CALC	sR EXP	$\delta\times10^5$	ID[b]	INT
10	0	(1172.09808)	------	---		0.
10	1	1172.08411	------	---		0.11E+00
10	2	1172.05141	------	---		0.11E+00
10	3	1171.94193	------	---		0.23E+00
10	4	1171.87637	------	---		0.12E+00
10	5	1171.77848	------	---		0.13E+00
10	6	1171.66235	------	---		0.29E+00
10	7	1171.60626	------	---		0.15E+00
10	8	1171.57537	------	---		0.16E+00
10	9	1171.62465	------	---		0.30E+00
10	10	1171.80295	------	---		0.11E+00
11	0	1190.14542	------	---		0.84E-01
11	1	1190.13081	------	---		0.42E-01
11	2	1190.10564	------	---		0.44E-01
11	3	1190.02263	------	---		0.92E-01
11	4	1189.90208	------	---		0.49E-01
11	5	1189.79110	------	---		0.53E-01
11	6	1189.67605	------	---		0.12E+00
11	7	1189.57286	------	---		0.65E-01
11	8	1189.50310	------	---		0.71E-01
11	9	1189.49665	------	---		0.15E+00
11	10	1189.59532	------	---		0.75E-01
11	11	1189.85772	------	---		0.57E-01
12	0	(1208.02220)	------	---		0.
12	1	1208.00689	------	---		0.15E-01
12	2	1208.00314	------	---		0.15E-01
12	3	1207.81930	------	---		0.32E-01
12	4	1207.75468	------	---		0.17E-01
12	5	1207.63009	------	---		0.19E-01
12	6	1207.49639	------	---		0.43E-01
12	7	1207.36748	------	---		0.24E-01
12	8	1207.26189	------	---		0.28E-01
12	9	1207.20488	------	---		0.63E-01
12	10	1207.23165	------	---		0.34E-01
12	11	1207.39173	------	---		0.35E-01
12	12	1207.75497	------	---		0.56E-01
13	0	1225.73480	------	---		0.94E-02
13	1	1225.71846	------	---		0.47E-02
13	2	1225.79286	------	---		0.49E-02
13	3	1225.60588	------	---		0.10E-01
13	4	1225.43754	------	---		0.56E-02
13	5	1225.29736	------	---		0.62E-02
13	6	1225.14359	------	---		0.14E-01
13	7	1224.98895	------	---		0.81E-02
13	8	1224.84938	------	---		0.94E-02
13	9	1224.74626	------	---		0.22E-01
13	10	1224.70887	------	---		0.13E-01
13	11	1224.77831	------	---		0.15E-01
13	12	1225.01282	------	---		0.31E-01
13	13	1225.49524	------	---		0.13E-01

TABLE II—*Continued*

		aP				
J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
1	0	(907.86748)	------	---		0.
2	0	888.31770	888.31765(50)	-4	H DL	0.47E+01
2	1	888.04159	888.04191(50)	32	B TC	0.18E+01
			888.04231(100)	72	H DL	
3	0	(869.06226)	------	---		0.
3	1	868.76671	------	---		0.23E+01
3	2	867.95232	------	---		0.15E+01
4	0	850.10666	------	---		0.45E+01
4	1	849.83322	------	---		0.22E+01
4	2	849.00592	------	---		0.18E+01
4	3	847.60137	------	---		0.23E+01
5	0	(831.44924)	------	---		0.
5	1	831.17937	------	---		0.17E+01
5	2	830.36421	------	---		0.15E+01
5	3	828.98061	------	---		0.25E+01
5	4	826.98946	------	---		0.81E+00
6	0	813.08212	------	---		0.22E+01
6	1	812.81699	------	---		0.11E+01
6	2	812.01864	------	---		0.11E+01
6	3	810.66343	------	---		0.20E+01
6	4	808.71454	------	---		0.82E+00
6	5	806.11607	------	---		0.53E+00
7	0	(794.99176)	------	---		0.
7	1	794.73225	------	---		0.64E+00
7	2	793.95497	------	---		0.63E+00
7	3	792.63655	------	---		0.12E+01
7	4	790.73896	------	---		0.57E+00
7	5	788.21099	------	---		0.49E+00
7	6	784.97969	------	---		0.64E+00
8	0	777.15998	------	---		0.66E+00
8	1	776.90666	------	---		0.33E+00
8	2	776.15424	------	---		0.33E+00
8	3	774.87605	------	---		0.67E+00
8	4	773.04150	------	---		0.33E+00
8	5	770.59608	------	---		0.31E+00
8	6	767.47180	------	---		0.54E+00
8	7	763.57776	------	---		0.18E+00
9	0	(759.56513)	------	---		0.
9	1	759.31814	------	---		0.15E+00
9	2	758.59395	------	---		0.16E+00
9	3	757.36663	------	---		0.32E+00
9	4	755.59714	------	---		0.16E+00
9	5	753.24432	------	---		0.16E+00
9	6	750.24008	------	---		0.32E+00
9	7	746.49791	------	---		0.14E+00
9	8	741.90665	------	---		0.98E-01
10	0	742.18335	------	---		0.13E+00
10	1	741.94230	------	---		0.64E-01
10	2	741.24935	------	---		0.66E-01
10	3	740.06716	------	---		0.14E+00
10	4	738.37837	------	---		0.70E-01
10	5	736.12605	------	---		0.73E-01
10	6	733.25213	------	---		0.15E+00
10	7	729.67494	------	---		0.75E-01
10	8	725.28929	------	---		0.69E-01

		aP				
J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
10	9	719.96170	------	---		0.58E-01
11	0	(724.99007)	------	---		0.
11	1	724.75376	------	---		0.24E-01
11	2	724.09496	------	---		0.25E-01
11	3	722.97704	------	---		0.52E-01
11	4	721.35670	------	---		0.27E-01
11	5	719.21046	------	---		0.29E-01
11	6	716.47425	------	---		0.62E-01
11	7	713.07156	------	---		0.33E-01
11	8	708.90367	------	---		0.34E-01
11	9	703.84498	------	---		0.63E-01
11	10	697.73728	------	---		0.23E-01
12	0	707.96156	------	---		0.16E-01
12	1	707.72736	------	---		0.82E-02
12	2	707.10613	------	---		0.84E-02
12	3	706.02864	------	---		0.16E-01
12	4	704.50431	------	---		0.94E-02
12	5	702.46724	------	---		0.10E-01
12	6	699.87302	------	---		0.22E-01
12	7	696.65065	------	---		0.12E-01
12	8	692.70819	------	---		0.13E-01
12	9	687.92839	------	---		0.28E-01
12	10	682.16314	------	---		0.14E-01
12	11	675.22675	------	---		0.10E-01
13	0	(691.07668)	------	---		0.
13	1	690.83882	------	---		0.25E-02
13	2	690.26075	------	---		0.26E-02
13	3	689.26100	------	---		0.55E-02
13	4	687.79571	------	---		0.29E-02
13	5	685.86832	------	---		0.32E-02
13	6	683.41716	------	---		0.72E-02
13	7	680.37700	------	---		0.40E-02
13	8	676.66303	------	---		0.45E-02
13	9	672.16667	------	---		0.10E-01
13	10	666.75035	------	---		0.55E-02
13	11	660.24110	------	---		0.55E-02
13	12	652.42254	------	---		0.66E-02

TABLE II—*Continued*

		aQ				
J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
0	0	(927.69900)	------	---		0.
1	0	(927.96073)	------	---		0.
1	1	927.69075	------	---		0.23E+01
2	0	(928.47697)	------	---		0.
2	1	928.21057	928.21042(30)	-14	H DL	0.10E+01
			928.21057(20)	0	C TN	
			928.21039(20)	-17	C TN	
2	2	927.40368	927.40348(20)	-19	C TN	0.44E+01
			927.40336(60)	-31	H DL	
3	0	(929.23368)	------	---		0.
3	1	928.97235	928.97235(20)	0	E HD	0.54E+00
			928.97280(50)	45	B TC	
3	2	928.18148	928.18153(20)	5	C TN	0.23E+01
			928.18148(20)	0	C TN	
			928.18184(100)	36	H DL	
3	3	926.83796	926.83752(20)	-43	C TC	0.11E+02
			926.83771(20)	-24	E HD	
			926.83761(40)	-34	H DL	
4	0	(930.21015)	------	---		0.
4	1	929.95528	929.95574(30)	46	H DL	0.28E+00
			929.95537(50)	9	B TC	
			929.95537(50)	9	B TC	
4	2	929.18523	929.18527(30)	4	H DL	0.12E+01
			929.18516(20)	-6	C TN	
			929.18536(20)	13	C TN	
4	3	927.87705	927.87716(20)	11	C TC	0.59E+01
4	4	925.99262	925.99240(20)	-21	A LN	0.59E+01
			925.99241(20)	-20	L LS	
			925.99242(30)	-19	H DL	
5	0	(931.38003)	------	---		0.
5	1	931.13269	931.13284(20)	15	H DL	0.14E+00
			931.13278(20)	9	E HD	
5	2	930.38788	930.38789(30)	1	H DL	0.60E+00
5	3	929.12281	929.12287(10)	6	A LC	0.30E+01
			929.12288(20)	7	C TN	
			929.12274(20)	-6	E HD	
			929.12315(20)	34	C TN	
5	4	927.29993	927.30030(120)	37	C TN	0.30E+01
			927.29996(10)	3	B LC	
5	5	924.86568	924.86560(20)	-7	C TN	0.55E+01
			924.86616(50)	48	B TC	
			924.86573(40)	5	H DL	
6	0	(932.71208)	------	---		0.
6	1	932.47307	------	---		0.68E-01
6	2	931.75743	931.75743(50)	0	H DL	0.28E+00
6	3	930.54102	930.54089(50)	-12	H DL	0.14E+01
			930.54024(60)	-77	H DL	
6	4	928.79026	928.79010(20)	-15	H DL	0.14E+01
			928.79067(50)	41	B TC	
			928.79037(20)	11	C TC	
			928.79018(20)	-7	E HD	
6	5	926.45139	------	---		0.26E+01
6	6	923.45408	923.45381(50)	-26	H DL	0.90E+01
			923.45354(100)	-53	A TN	
			923.45401(40)	-6	H DL	

		aQ				
J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
7	0	(934.17133)	------	---		0.
7	1	933.94108	933.94143(40)	35	H DL	0.30E-01
7	2	933.25804	933.25821(50)	17	H DL	0.13E+00
7	3	932.09881	932.09898(20)	17	C TC	0.62E+00
7	4	930.42538	930.42521(30)	-16	H DL	0.62E+00
7	5	928.19279	928.19268(30)	-10	H DL	0.11E+01
7	6	925.33187	925.33241(100)	54	A TN	0.40E+01
7	7	921.75374	921.75343(20)	-30	L LS	0.34E+01
			921.75374(50)	0	C TC	
			921.75469(50)	95	B TC	
8	0	(935.72030)	------	---		0.
8	1	935.49882	------	---		0.12E-01
8	2	934.85134	934.85127(20)	-6	C TC	0.51E-01
			934.85121(20)	-12	E HD	
8	3	933.74686	933.74676(50)	-9	H DL	0.25E+00
8	4	932.16423	------	---		0.25E+00
8	5	930.04671	930.04696(20)	25	C TC	0.46E+00
			930.04671(50)	0	B TC	
			930.04654(20)	-16	C TN	
			930.04702(70)	31	H DL	
8	6	927.33364	927.33375(20)	11	H DL	0.16E+01
8	7	923.94075	923.94090(20)	15	C TN	0.14E+01
			923.94084(20)	9	C TC	
8	8	919.75951	919.76057(60)	106	H DL	0.24E+01
9	0	(937.32042)	------	---		0.
9	1	937.10717	------	---		0.46E-02
9	2	936.49784	------	---		0.19E-01
9	3	935.46630	------	---		0.95E-01
9	4	933.96440	933.96415(20)	-24	C TC	0.95E-01
			933.96508(80)	68	H DL	
9	5	931.96851	931.96844(20)	-6	C TC	0.17E+00
9	6	929.41188	929.41177(20)	-10	C TN	0.61E+00
			929.41222(80)	34	H DL	
9	7	926.21526	------	---		0.52E+00
9	8	922.27640	------	---		0.68E+00
9	9	917.46527	917.46528(20)	1	C TN	0.30E+01
			917.46532(20)	5	C TN	
10	0	(938.93353)	------	---		0.
10	1	938.72717	------	---		0.16E-02
10	2	938.15845	------	---		0.67E-02
10	3	937.17273	------	---		0.33E-01
10	4	935.78374	------	---		0.33E-01
10	5	933.91361	933.91389(40)	28	H DL	0.60E-01
10	6	931.51900	931.51834(50)	-65	H DL	0.21E+00
10	7	928.52599	928.52549(30)	-49	H DL	0.18E+00
			928.52593(20)	-5	C TN	
10	8	924.83904	924.83897(20)	-6	C TC	0.30E+00
10	9	920.33628	920.33622(20)	-5	C TN	0.10E+01
			920.33626(20)	-1	C TN	
			920.33583(20)	-44	L LS	
10	10	914.86383	------	---		0.90E+00
11	0	(940.52347)	------	---		0.
11	1	940.32123	------	---		0.51E-03
11	2	939.79608	------	---		0.21E-02
11	3	938.91054	------	---		0.11E-01

TABLE II—*Continued*

sQ

J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
11	4	937.58193	------	---		0.11E-01
11	5	935.83921	------	---		0.19E-01
11	6	933.60905	933.60880(50)	-24	H DL	0.67E-01
11	7	930.82319	930.82348(20)	29	C TC	0.57E-01
			930.82286(20)	-32	E HD	
11	8	927.39307	927.39273(30)	-33	H DL	0.57E-01
11	9	923.20543	923.20616(20)	73	C TN	0.33E+00
			923.20546(20)	3	C TN	
			923.20502(20)	-40	L LS	
11	10	918.11687	------	---		0.28E+00
11	11	911.94699	------	---		0.50E+00
12	0	(942.05777)	------	---		0.
12	1	941.85372	------	---		0.15E-03
12	2	941.37731	------	---		0.63E-03
12	3	940.49827	------	---		0.31E-02
12	4	939.32225	------	---		0.31E-02
12	5	937.70600	------	---		0.56E-02
12	6	935.63951	------	---		0.20E-01
12	7	933.06040	933.06067(20)	27	H DL	0.17E-01
			933.06019(20)	-20	C TN	
			933.06062(20)	22	E HD	
12	8	929.88738	929.88748(40)	10	H DL	0.28E-01
12	9	926.01610	926.01606(40)	-3	H DL	0.96E-01
12	10	921.31397	921.31381(20)	-15	C TN	0.83E-01
12	11	915.61375	------	---		0.14E+00
12	12	908.70549	908.70549(20)	0	L LS	0.52E+00
13	0	(943.50939)	------	---		0.
13	1	943.28785	------	---		0.40E-04
13	2	942.87415	------	---		0.17E-03
13	3	942.15404	------	---		0.63E-03
13	4	940.97327	------	---		0.83E-03
13	5	939.47993	------	---		0.15E-02
13	6	937.57306	------	---		0.53E-02
13	7	935.19635	------	---		0.45E-02
13	8	932.27597	------	---		0.75E-02
13	9	928.71671	928.71692(30)	21	H DL	0.26E-01
			928.71667(20)	-3	C TN	
13	10	924.39710	------	---		0.22E-01
13	11	919.16327	919.16452(80)	125	H DL	0.38E-01
13	12	912.82153	------	---		0.14E+00
13	13	905.12900	------	---		0.13E+00
14	9	931.26278	931.26264(30)	-13	H DL	0.63E-02
14	10	927.31530	------	---		0.54E-02
14	11	922.53716	------	---		0.94E-02
14	12	916.75104	916.75101(20)	-2	C TN	0.33E-01
14	13	909.73388	------	---		0.30E-01
15	9	933.61880	933.61787(100)	-92	H DL	0.14E-02
15	10	930.02673	------	---		0.12E-02
15	11	925.68626	925.68652(50)	26	H DL	0.21E-02

sR

J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
0	0	947.79225	947.79201(20)	-23	E HD	0.33E+01
1	0	(968.12000)	------	---		0.
1	1	967.85973	967.85956(20)	-16	C TC	0.24E+01
			967.86020(100)	47	A TC	
			967.85889(100)	-83	H DL	
2	0	988.64840	------	---		0.78E+01
2	1	988.39621	988.39620(20)	0	C TC	0.35E+01
2	2	987.63285	987.63283(10)	-1	A LC	0.23E+01
3	0	(1009.33718)	------	---		0.
3	1	1009.09441	------	---		0.38E+01
3	2	1008.36078	------	---		0.32E+01
3	3	1007.11364	------	---		0.41E+01
4	0	1030.14093	------	---		0.69E+01
4	1	1029.90860	------	---		0.34E+01
4	2	1029.20890	1029.20904(20)	14	C TC	0.31E+01
4	3	1028.01924	------	---		0.52E+01
4	4	1026.30308	1026.30329(20)	21	C TC	0.17E+01
5	0	(1051.00998)	------	---		0.
5	1	1050.78878	------	---		0.26E+01
5	2	1050.12666	1050.12685(20)	19	C TC	0.25E+01
5	3	1049.00040	------	---		0.46E+01
5	4	1047.37565	1047.37583(20)	18	C TC	0.19E+01
5	5	1045.20101	1045.20105(20)	4	E HD	0.12E+01
			1045.20087(20)	-13	L LS	
6	0	1071.89165	1071.89155(20)	-9	E HD	0.35E+01
6	1	1071.68189	1071.68213(20)	24	C TC	0.17E+01
6	2	1071.06049	------	---		0.17E+01
6	3	1070.00328	------	---		0.33E+01
6	4	1068.47669	------	---		0.15E+01
6	5	1066.43318	1066.43348(20)	30	C TC	0.13E+01
6	6	1063.80627	------	---		0.17E+01
7	0	(1092.73165)	------	---		0.
7	1	1092.53324	------	---		0.10E+01
7	2	1091.95513	------	---		0.10E+01
7	3	1090.96963	1090.96955(20)	-7	C TC	0.21E+01
			1090.96971(50)	8	B TC	
7	4	1089.54811	------	---		0.10E+01
7	5	1087.64342	1087.64349(20)	7	C TC	0.97E+00
7	6	1085.19372	------	---		0.17E+01
7	7	1082.11672	1082.11719(20)	47	E HD	0.57E+00
			1082.11772(20)	100	C TC	
8	0	1113.47559	------	---		0.11E+01
8	1	1113.28786	------	---		0.55E+00
8	2	1112.75524	------	---		0.56E+00
8	3	1111.84653	------	---		0.11E+01
8	4	1110.53149	------	---		0.58E+00
8	5	1108.77090	------	---		0.58E+00
8	6	1106.50545	------	---		0.11E+01
8	7	1103.65809	------	---		0.51E+00
8	8	1100.12927	------	---		0.36E+00
9	0	(1134.07060)	------	---		0.
9	1	1133.89205	------	---		0.26E+00
9	2	1133.40695	------	---		0.27E+00
9	3	1132.57188	------	---		0.55E+00
9	4	1131.36978	------	---		0.29E+00

TABLE II—*Continued*

		aR				
J	K	CALC	EXP	$\delta \times 10^5$	ID[b]	INT
9	5	1129.75607	------	---		0.30E+00
9	6	1127.67874	------	---		0.62E+00
9	7	1125.06631	------	---		0.31E+00
9	8	1121.82615	------	---		0.29E+00
9	9	1117.83984	------	---		0.41E+00
10	0	1154.46693	------	---		0.22E+00
10	1	1154.29465	------	---		0.11E+00
10	2	1153.85957	------	---		0.12E+00
10	3	1153.10623	------	---		0.24E+00
10	4	1152.00897	------	---		0.13E+00
10	5	1150.54236	------	---		0.14E+00
10	6	1148.65380	------	---		0.29E+00
10	7	1146.27762	------	---		0.16E+00
10	8	1143.32644	------	---		0.16E+00
10	9	1139.69673	------	---		0.31E+00
10	10	1135.24342	------	---		0.11E+00
11	0	(1174.61968)	------	---		0.
11	1	1174.44759	------	---		0.44E-01
11	2	1174.06726	------	---		0.45E-01
11	3	1173.38016	------	---		0.95E-01
11	4	1172.39988	------	---		0.51E-01
11	5	1171.07797	------	---		0.55E-01
11	6	1169.37554	------	---		0.12E+00
11	7	1167.23295	------	---		0.67E-01
11	8	1164.57226	------	---		0.73E-01
11	9	1161.29314	------	---		0.16E+00
11	10	1157.26770	------	---		0.76E-01
11	11	1152.33398	------	---		0.58E-01
12	0	1194.49048	------	---		0.30E-01
12	1	1194.30276	------	---		0.15E-01
12	2	1193.99071	------	---		0.16E-01
12	3	1193.39131	------	---		0.34E-01
12	4	1192.49982	------	---		0.18E-01
12	5	1191.31761	------	---		0.20E-01
12	6	1189.79542	------	---		0.44E-01
12	7	1187.87976	------	---		0.25E-01
12	8	1185.50032	------	---		0.28E-01
12	9	1182.56614	------	---		0.64E-01
12	10	1178.96072	------	---		0.35E-01
12	11	1174.53592	------	---		0.36E-01
12	12	1169.10448	------	---		0.56E-01
13	0	(1214.04912)	------	---		0.
13	1	1213.77715	------	---		0.49E-02
13	2	1213.59861	------	---		0.51E-02
13	3	1213.04222	------	---		0.11E-01
13	4	1212.27431	------	---		0.59E-02
13	5	1211.22425	------	---		0.65E-02
13	6	1209.87321	------	---		0.15E-01
13	7	1208.17389	------	---		0.84E-02
13	8	1206.06378	------	---		0.98E-02
13	9	1203.46136	------	---		0.23E-01
13	10	1200.26162	------	---		0.13E-01
13	11	1196.33038	------	---		0.15E-01
13	12	1191.49721	------	---		0.31E-01
13	13	1185.54672	------	---		0.13E-01

[a] CALC and EXP are calculated and observed transition wavenumbers, δ = EXP - CALC.

[b] Symbols given in this column identify the authors of the corresponding measurement and the technique used: A ref.(8); B ref.(9); C ref.(10); E refs.(12,13); F ref.(20); H our measurement; L ref.(11). Experimental techniques are denoted by the following symbols: HD diode laser heterodyne, DL standard diode laser, LS laser Stark spectroscopy; TC and TN are two photon infrared-microwave techniques with CO_2 and N_2O lasers, respectively; LC and LN are two-photon infrared-microwave techniques using the Lamb-dip effect.

[c] This value has not been taken into the fit.

TABLE III

Ground State and ν_2 Excited State Molecular Parameters of $^{15}NH_3$ (cm^{-1})[a]

Parameter[b]	Ground-State Value	ν_2 -State Value	Parameter[b]	Ground-State Value	ν_2 -State Value
ΔE_0	0.7576868(13)	34.437785(16)	$^{(s)}E_0$	0.[c]	928.456683(76)[d]
ΔB	$-4.92922(13)\times10^{-3}$	-0.1777943(51)	$^{(s)}B$	9.9223556(24)	10.0489023(65)
$\Delta(C-B)$	$6.85128(16)\times10^{-3}$	0.2474842(80)	$^{(s)}C-^{(s)}B$	-3.700(13)	-3.964(14)
ΔD_J	$-1.67575(45)\times10^{-5}$	$-0.43867(21)\times10^{-3}$	$^{(s)}D_J$	$0.85167(30)\times10^{-3}$	$1.13920(38)\times10^{-3}$
ΔD_{JK}	$4.60854(100)\times10^{-5}$	$1.19920(55)\times10^{-3}$	$^{(s)}D_{JK}$	$-1.5832(12)\times10^{-3}$	$-2.4427(12)\times10^{-3}$
ΔD_K	$-3.14644(61)\times10^{-5}$	$-0.81075(53)\times10^{-3}$	$^{(s)}D_K$	$1.\times10^{-3}$ [c]	$1.61535(70)\times10^{-3}$
ΔH_{JJJ}	$-0.40575(65)\times10^{-7}$	$-0.6501(29)\times10^{-6}$	$^{(s)}H_{JJJ}$	$0.2546(35)\times10^{-6}$	$0.5534(53)\times10^{-6}$
ΔH_{JJK}	$1.6538(22)\times10^{-7}$	$2.599(11)\times10^{-6}$	$^{(s)}H_{JJK}$	$-0.907(17)\times10^{-6}$	$-2.236(24)\times10^{-6}$
ΔH_{JKK}	$-2.2307(26)\times10^{-7}$	$-3.396(17)\times10^{-6}$	$^{(s)}H_{JKK}$	$1.125(35)\times10^{-6}$	$2.978(41)\times10^{-6}$
ΔH_{KKK}	$0.99622(101)\times10^{-7}$	$1.463(12)\times10^{-6}$	$^{(s)}H_{KKK}$	-0.5×10^{-6} [c]	$-1.320(14)\times10^{-6}$
ΔG_{JJJJ}	$0.7608(42)\times10^{-10}$	$0.564(13)\times10^{-9}$	$^{(s)}G_{JJJJ}$	$-0.982(102)\times10^{-10}$	$-0.183(24)\times10^{-9}$
ΔG_{JJJK}	$-4.110(20)\times10^{-10}$	$-2.877(70)\times10^{-9}$	$^{(s)}G_{JJJK}$	$5.68(60)\times10^{-10}$	$1.20(13)\times10^{-9}$
ΔG_{JJKK}	$8.248(36)\times10^{-10}$	$5.29(16)\times10^{-9}$	$^{(s)}G_{JJKK}$	$-12.1(12)\times10^{-10}$	$-2.60(28)\times10^{-9}$
ΔG_{JKKK}	$-7.296(27)\times10^{-10}$	$-4.23(19)\times10^{-9}$	$^{(s)}G_{JKKK}$	$10.0(11)\times10^{-10}$	$2.17(26)\times10^{-9}$
ΔG_{KKKK}	$2.4013(78)\times10^{-10}$	$1.253(100)\times10^{-9}$	$^{(s)}G_{KKKK}$	$-1.\times10^{-10}$ [c]	$-0.436(90)\times10^{-9}$
ΔL_{JJJJJ}	$-0.8737(102)\times10^{-13}$	0. [c]	η_3^0	$4.2650(38)\times10^{-9}$	$1.709(38)\times10^{-9}$
ΔL_{JJJJK}	$5.909(64)\times10^{-13}$	0. [c]	η_3^J	$-4.947(15)\times10^{-12}$	0. [c]
ΔL_{JJJKK}	$-15.81(15)\times10^{-13}$	0. [c]	η_6^0	$1.73(24)\times10^{-19}$	0. [c]
ΔL_{JJKKK}	$20.92(18)\times10^{-13}$	0. [c]	α^0	8.0×10^{-5} [c]	$1.2940(49)\times10^{-4}$
ΔL_{JKKKK}	$-13.715(104)\times10^{-13}$	0. [c]			
ΔL_{KKKKK}	$3.565(24)\times10^{-13}$	0. [c]			

[a] Values in parentheses are standard deviations of the parameters, given in units of the last digit quoted.

[b] If X denotes a general parameter, ΔX is defined as $\Delta X = {}^{(a)}X - {}^{(s)}X$, where ${}^{(a)}X$ is the parameter referring to the upper level of the inversion doublet; ΔE_0 is the inversion splitting in the ground and ν_2 excited state for $J = K = 0$; η and α are parameters describing the $\Delta k = \pm 3n$ interactions [refs.(1,2,4)].

[c] Constrained value.

[d] Band origin for the $a \leftarrow s$ transition is $962.894468(92)\,cm^{-1}$, for the $s \leftarrow a$ transition is $927.698996(77)\,cm^{-1}$.

It should also be noted that the diode laser data of $^{15}NH_3$ in Table II (obtained by using $^{14}NH_3$ as a calibration standard) are highly consistent with the other precise ν_2 band data. This confirms that the $^{14}NH_3$ ν_2 band wavenumbers (*2*) can be used as a reliable calibration standard.

It is obvious from a comparison of the spectroscopical parameters of $^{14}NH_3$ [Table III in Ref. (*2*)] and $^{15}NH_3$ (Table III in this paper), that there is a close correspondence between all of the $^{14}NH_3$ and $^{15}NH_3$ molecular parameters. Such a correspondence can be expected but the fact that we did arrive at it seems to indicate that the $^{14}NH_3$ and $^{15}NH_3$ data sets are consistent.

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