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High-Resolution Fourier Transform and Submillimeter-wave Study of the ν_6 Band of $^{12}CH_3F$

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The ν_6 band of $^{12}CH_3F$ has been measured in the range 1077–1278 cm^{-1} using a Fourier transform spectrometer with a resolution of 0.002 cm^{-1}. The wavenumbers of 1070 rovibrational transitions have been used simultaneously with 99 previously reported frequencies of the ground state rotational transitions and 135 frequencies of rotational transitions in the $v_6 = 1$ excited vibrational state to determine 24 parameters of the ν_6 band and 6 spectroscopic parameters of the ground vibrational state of $^{12}CH_3F$.

I. INTRODUCTION

The ν_6 band of $^{12}CH_3F$ consists of the $\Delta v_6 = 1$, $\Delta J = 0, \pm 1$, $\Delta K = \pm 1$ rovibrational transitions to the doubly degenerate vibrational level of the CH_3 rocking mode. Smith and Mills (*1*) recorded this band with 0.25-cm^{-1} resolution, resolved partly the J and K structure of the band, and observed intensity perturbations in the rotational lines.

The first high-resolution study of this band was the diode laser measurement of five Q branches, done by Hirota (*2*). Cho *et al.* (*3*) used the infrared-microwave sideband laser spectrometer to measure the $\nu_3 + \nu_6 - \nu_6$ band of $^{12}CH_3F$ and determined the spectroscopic parameters of the $v_6 = 1$ state from about 200 transitions with J and K values up to 20 and 10, respectively.

In this paper, we report the measurement and analysis of the high-resolution Fourier transform spectra of the ν_6 band of $^{12}CH_3F$, recorded at Doppler limited resolution with the Bruker IFS 120 HR spectrometer at the University of Giessen (*4*). We have

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also measured pure rotational transition frequencies in the ground and $v_6 = 1$ vibrational states of $^{12}CH_3F$ using the submillimeter-wave RAD3 spectrometer with acoustic detection which was built at the Institute of Applied Physics in Nizhnii Novgorod (formerly Gorkii) (*5*).

The ν_6 band of $^{12}CH_3F$ is an ideal example for testing different reduction schemes of effective rotational Hamiltonians developed for degenerate vibrational states of symmetric top molecules (*6–8*) which are not strongly perturbed by Coriolis interactions with other vibrational states. This is a problem of the determinability of various spectroscopic parameters in the effective rotational Hamiltonians, which will be discussed in more detail in Sections III and IV of this paper.

Last but not least, methyl fluoride has been used for various laser spectroscopic experiments [see, e.g., Ref. (*9*) and the references cited therein] and for experiments with optically pumped submillimeter-wave lasers [see, e.g., Ref. (*10*)]. These experiments were based on the near coincidence of methyl fluoride ν_3 band transition frequencies with CO_2 laser frequencies. The data base of the precise line positions of the ν_6 band may be useful for extending these studies to another spectral region.

II. EXPERIMENTAL DETAILS

The sample of $^{12}CH_3F$ was prepared by the reaction of the methyl ester of perfluorosulfonic acid with NaF according to Edgell and Parts (*11*). Methyl fluoride was obtained by distillation at the temperature of a bath of solid CO_2 and ethyl alcohol as a fraction with the boiling point −78°C. Its purity was checked by the GC-MS technique.

The Fourier transform spectrum of the ν_6 band was measured with the Bruker IFS 120 HR spectrometer. The sample pressure was 50 Pa (=0.375 Torr) and the path length was 284 cm at a temperature of 300 K.

After finishing the CH_3F measurement, the cell of the Bruker IFS 120 HR spectrometer was evacuated and the N_2O spectrum was measured at 50 Pa in the range 1130–1220 cm^{-1}. Ten lines of the N_2O band were chosen in this range for calibration purposes; i.e., a correction factor was determined by fitting the differences between the measured N_2O line positions and those given in Ref. (*12*). The measured CH_3F line positions were then multiplied by this factor to obtain corrected line positions. The signal to noise ratio was determined to be 70.

The frequencies of the pure rotational transitions in the $v_6 = 1$ state of $^{12}CH_3F$ were measured with the RAD spectrometer (*5*) at room temperature and at sample pressures varying from 25 to 50 Pa.

III. THEORY

Energy Levels

In this paper, we will treat the ν_6 band of $^{12}CH_3F$ as an isolated band; i.e., we will assume that all the vibration–rotation interactions off-diagonal in the principle vibrational quantum numbers v_i can be described by the effective values of spectroscopic parameters of the $v_6 = 1$ state (*13*). The expression for the rovibrational term values can be then written as

$$
\begin{aligned}
E_v(J, K; l)/hc = {} & E_v^0/hc + B_6 J(J+1) + (A_6 - B_6)K^2 \\
& + [-2(A\zeta^z)_6 Kl + \eta_J J(J+1)Kl + \eta_K K^3 l + \tau_J J^2(J+1)^2 Kl \\
& + \tau_{JK} J(J+1)K^3 l + \tau_K K^5 l + \sigma_J J^3(J+1)^3 Kl + \sigma_{JK} J^2(J+1)^2 K^3 l \\
& + \sigma_{KJ} J(J+1)K^5 l + \sigma_K K^7 l + \cdots] \\
& + \{D_J J^2(J+1)^2 - D_{JK} J(J+1)K^2 - D_K K^4 + H_J J^3(J+1)^3 \\
& + H_{JK} J^2(J+1)^2 K^2 + H_{KJ} J(J+1)K^4 + H_K K^6 \\
& + L_J J^4(J+1)^4 + L_{JJK} J^3(J+1)^3 K^2 + L_{JK} J^2(J+1)^2 K^4 \\
& \qquad + L_{KKJ} J(J+1)K^6 + L_K K^8 + \cdots\} + E_{\text{off-d}}/hc, \quad (1)
\end{aligned}
$$

where $l = +1$ for the $+l$ levels and $l = -1$ for the $-l$ levels of the $v_6 = 1$ state.

The term $E_{\text{off-d}}/hc$ represents corrections to the rovibrational term value due to the terms in the expanded Hamiltonian of a C_{3v} molecule which are diagonal in v but off-diagonal in l. $E_{\text{off-d}}$ consists of several terms; the most important are considered here [cf. Ref. (*14*)].

(i) The $\Delta l = \pm 2$, $\Delta k = \pm 2$ interaction ("2,2" l-type interaction) has a diagonal contribution to the $kl = +1$ level of the $v_6 = 1$ state:

$$
\begin{aligned}
\langle A_\pm^{(1)} | (H_{22} + H_{24})/hc | A_\pm^{(1)} \rangle & [\equiv E_l(J, kl = 1)/hc] \\
& = \pm 2[(q_{22} + 2f_{22}^{(K)}) + f_{22}^{(J)} J(J+1)]J(J+1), \quad (2)
\end{aligned}
$$

where, using the basis functions $|v^l; J, k\rangle$,

$$|A_\pm^{(1)}\rangle = 2^{-1/2}[|1^{+1}; J, +1\rangle \pm |1^{-1}; J, -1\rangle]. \quad (3)$$

This interaction has the following off-diagonal contribution to the $kl \neq 1$ levels, as obtained by a second-order perturbation treatment:

$$
\begin{aligned}
E_l(J, K \pm 1; \pm l) = {} & \pm[(q_{22} + 2f_{22}^{(K)}) + f_{22}^{(J)} J(J+1) + 2f_{22}^{(K)} K^2] \\
& \times [J(J+1) - K(K+1)][J(J+1) - K(K-1)]/[A_6 - B_6 - (A\zeta^z)_6]K, \quad (4)
\end{aligned}
$$

where all the signs on both sides of this equation are correlated.

In deriving these results, we used the same phase convention for the wavefunctions as Di Lonardo *et al.* (*14*) in their expressions for the matrix elements of various higher-order terms in the expanded rovibrational Hamiltonian.

(ii) The $\Delta l = \pm 2$, $\Delta k = \mp 4$ interaction has the following diagonal contribution to the $kl = -2$ levels in the $v_6 = 1$ state:

$$\langle A_\pm^{(2)} | H_{24}/hc | A_\pm^{(2)} \rangle = \pm 2[f_{24} + f_{24}^{(J)} J(J+1)][J(J+1) - 2][J(J+1)], \quad (5)$$

where

$$|A_\pm^{(2)}\rangle = 2^{-1/2}[|1^{+1}; J, -2\rangle \pm |1^{-1}; J; +2\rangle]. \quad (6)$$

This interaction leads to the A_1–A_2 splitting of the $kl = -2$ levels which was resolved for high J values in the ${}^PP_3(J)$, ${}^PQ_3(J)$, and ${}^PR_3(J)$ branches of the ν_6 band (Fig. 1).

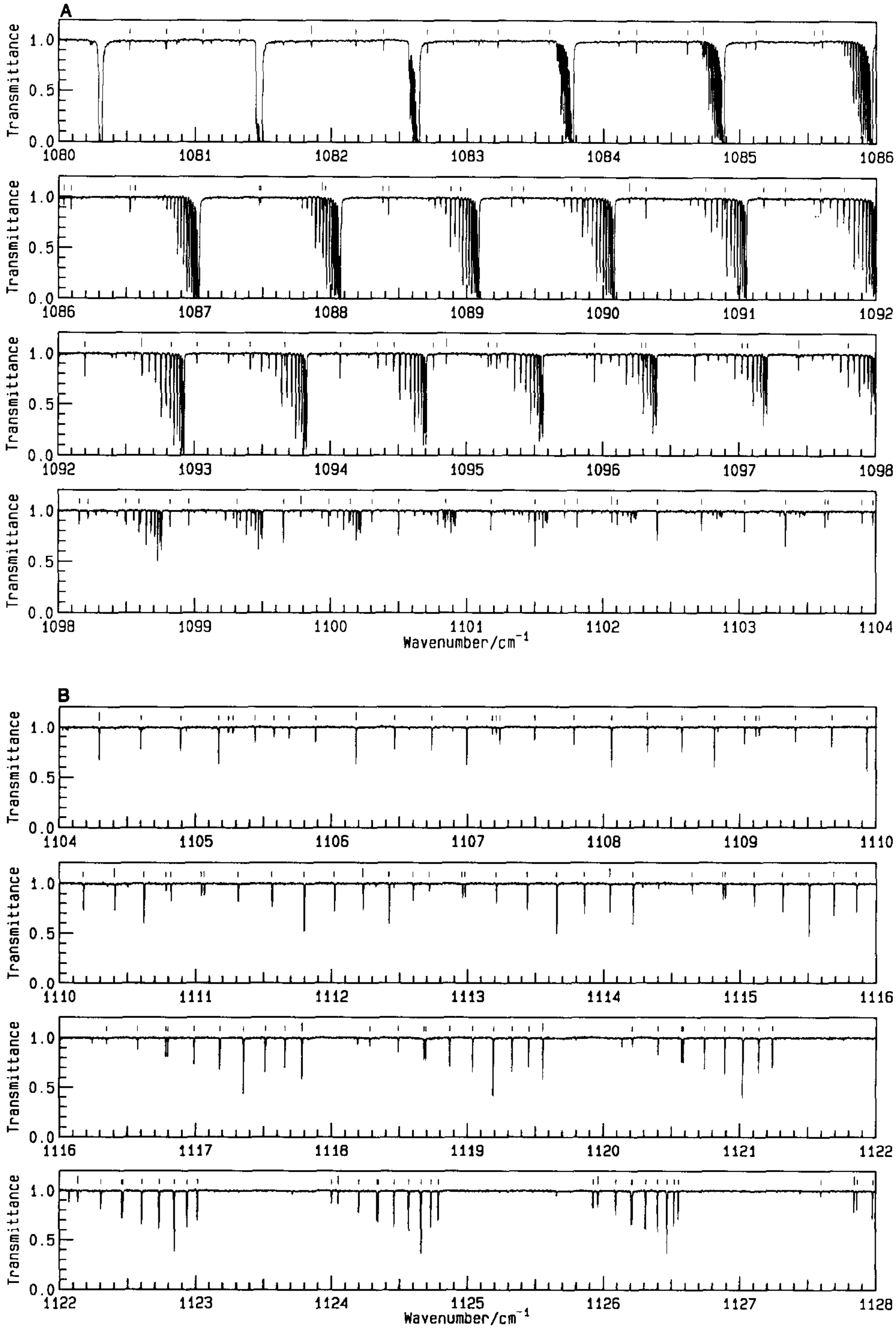


FIG. 1. Plot of the FT-IR spectrum of the ν_6 band of $^{12}CH_3F$ between 1080 and 1272 cm^{-1}. Vertical lines above the spectrum denote assigned transitions of this band, and longer lines correspond to transitions whose numbers in the list (see Table A1) are multiples of 10.

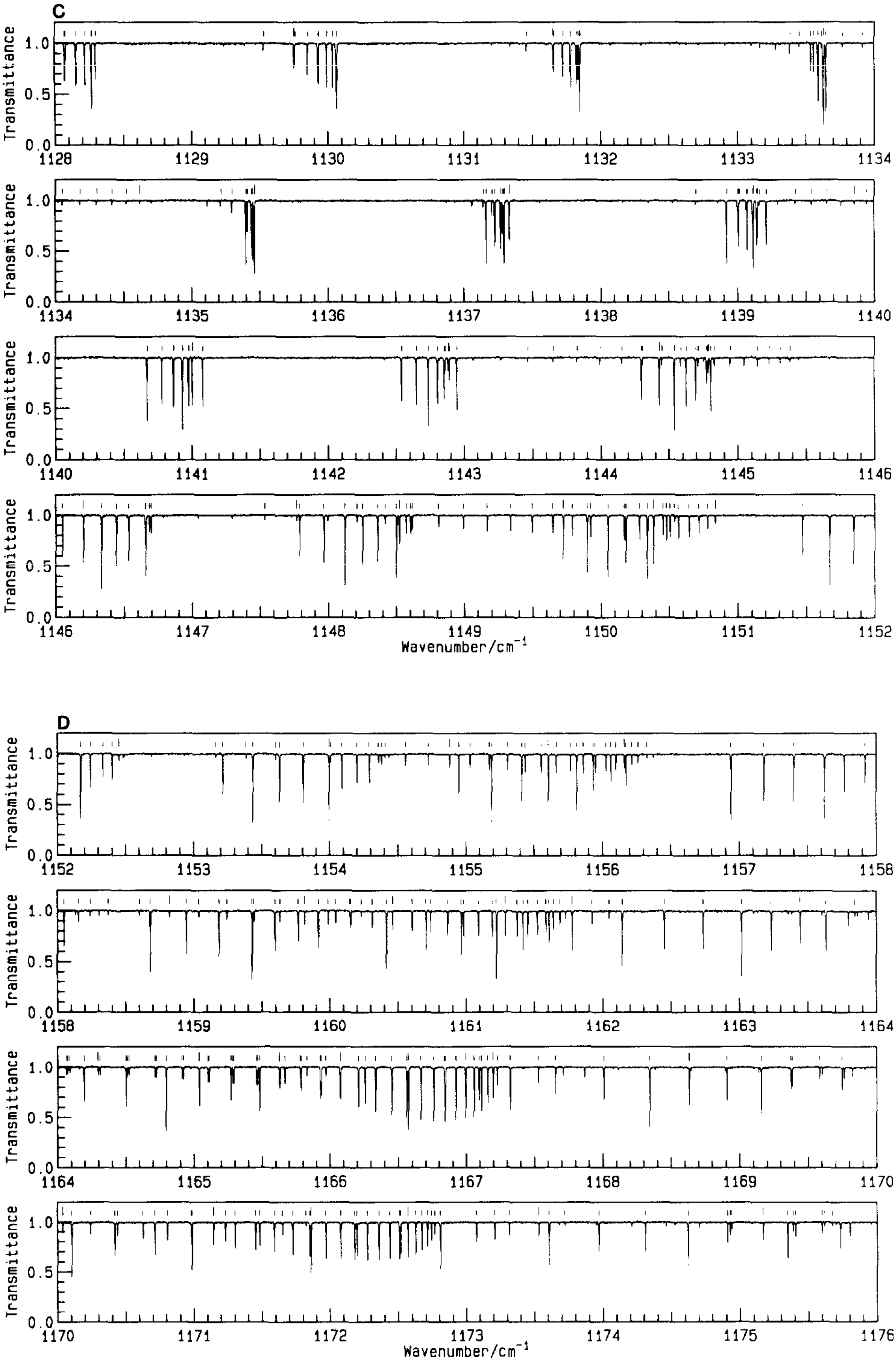


FIG. 1—*Continued*

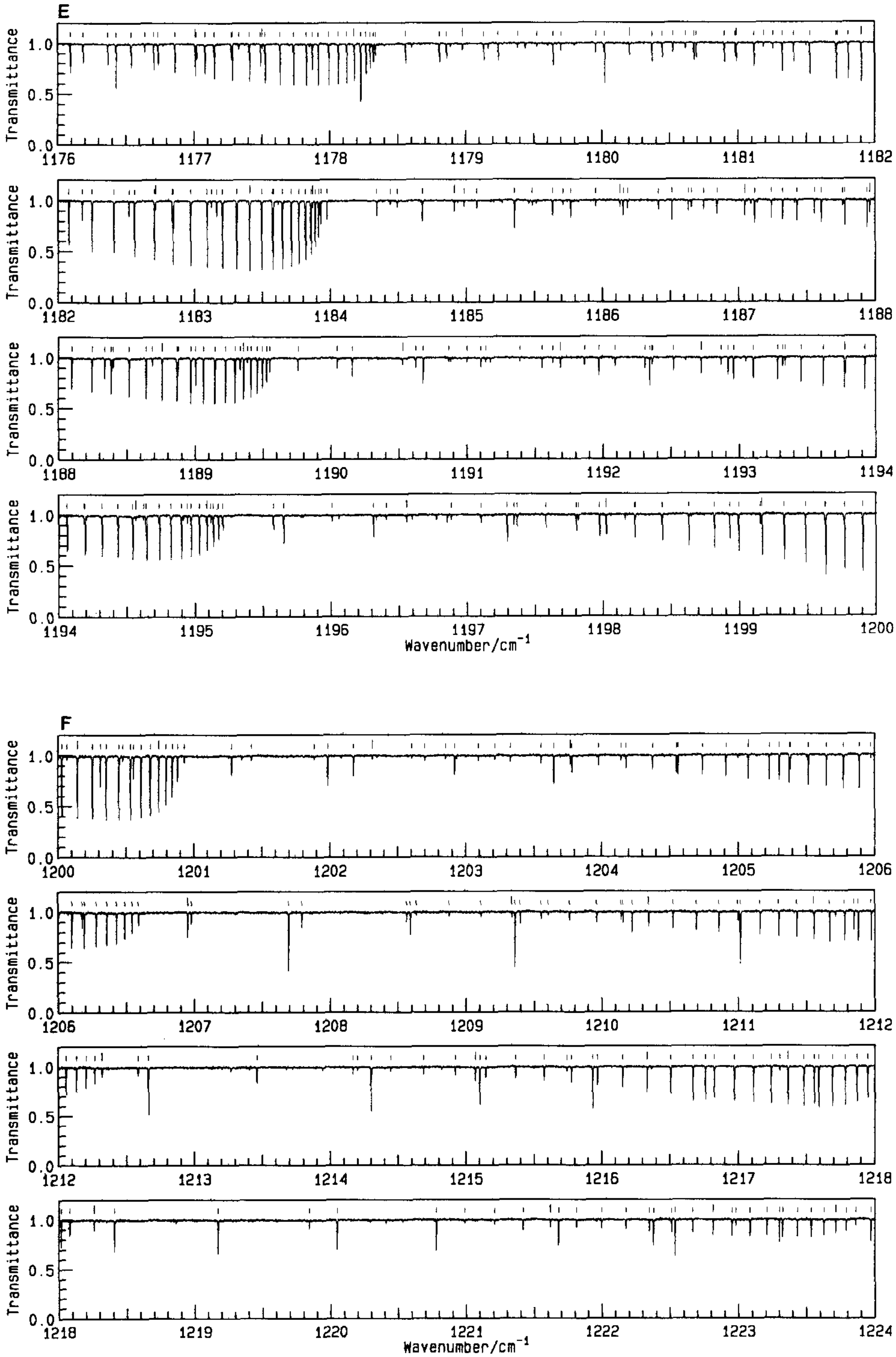
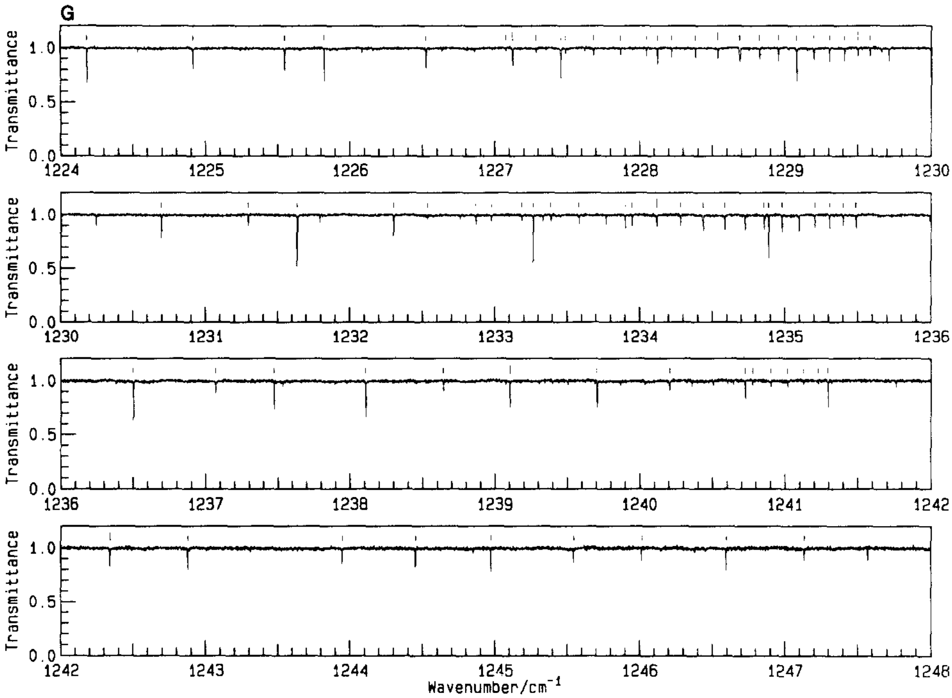


FIG. 1—*Continued*



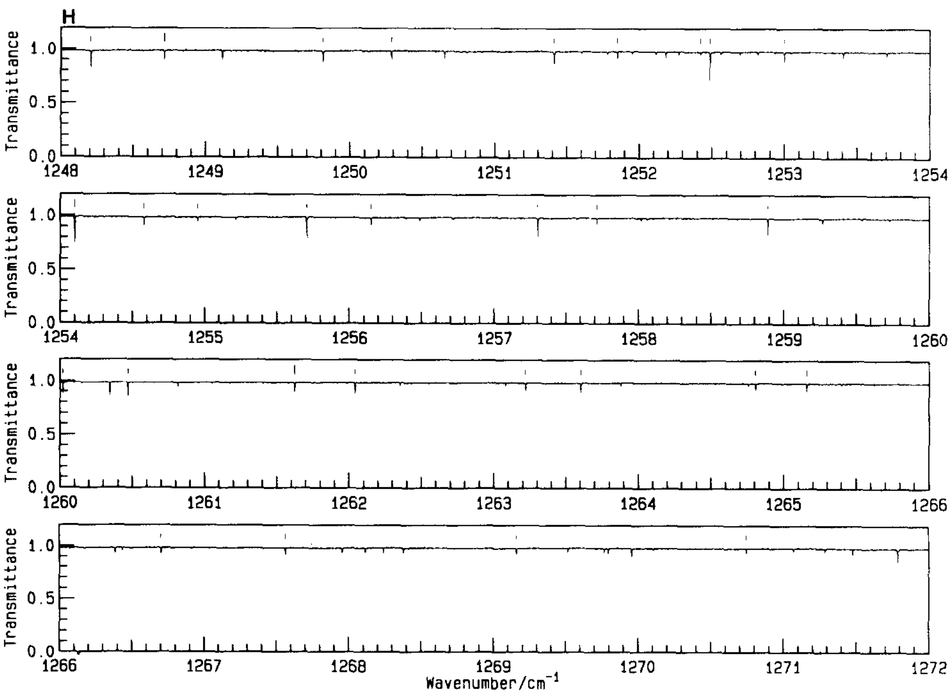


FIG. 1—*Continued*

On the other hand, the contribution of the off-diagonal matrix elements of this interaction was found to be negligible even for the microwave accuracy of the experiment.

(iii) The $\Delta l = \pm 2$, $\Delta k = \mp 1$ interaction (the "2,−1" l-type interaction) has purely off-diagonal contributions to the term values due to the matrix elements

$$\langle 1^{-1}; J, k+1 | (H_{22} + H_{24})/hc | 1^{+1}; J, k \rangle = 2\{[q_{12} + f_{12}^{(J)} J(J+1)] \times (2k+1) + f_{12}^{(K)}[k^3 + (k+1)^3]\}[J(J+1) - k(k+1)]^{1/2}. \quad (7)$$

The parameters q_{12} and $f_{12}^{(J)}$ can be shown to be completely correlated with other parameters [cf. Ref. (*8*)] and cannot be determined by fitting the experimental data.

The $\Delta v = \Delta l = 0$, $\Delta k = \pm 3$ interactions [ϵ parameters in Table II of Ref. (*14*)] are extremely small in the ground and $v_6 = 1$ states of $^{12}CH_3F$ and have not been taken into account in this paper. Thus if we put $E_v^0 = 0$, $E_{\text{off-d}} = 0$, and $l = 0$ in Eq. (1), we obtain the expression for the ground state energy levels of $^{12}CH_3F$.

Line Positions

If we apply the usual selection rules $\Delta J = 0, \pm 1$ and $\Delta K = \pm 1$ for $\Delta l = \pm 1$ transitions, employ Eq. (1), and collect terms with the same J, K, and l dependence, we obtain expressions for the wavenumbers ν of the rovibrational transitions in terms of the new effective parameters X^*.

$$\begin{aligned}\nu_{vr}(J, K; \Delta l) = {} & E_v^* + B_6^* J'(J'+1) + (A_6 - B_6)^* K^2 \\ & + [-2(A\zeta^z)_6^* Kl + \eta_J^* J'(J'+1)Kl + \eta_K^* K^3 l + \tau_J^* J'^2(J'+1)^2 Kl \\ & + \tau_{JK}^* J'(J'+1)K^3 l + \tau_K^* K^5 l + \sigma_J^* J'^3(J'+1)^3 Kl \\ & + \sigma_{JK}^* J'^2(J'+1)^2 K^3 l + \sigma_{KJ}^* J'(J'+1)K^5 l + \sigma_K^* K^7 l + \cdots] \\ & + [-D_J^* J'^2(J'+1)^2 - D_{JK}^* J'(J'+1)K^2 - D_K^* K^4 + H_J^* J'^3(J'+1)^3 \\ & + H_{JK}^* J'^2(J'+1)^2 K^2 + H_{KJ}^* J'(J'+1)K^4 + H_K^* K^6 \\ & + L_J^* J'^4(J'+1)^4 + L_{JJK}^* J'^3(J'+1)^3 K^2 + \cdots] \\ & + \Delta E_l^*(J', K)/hc - E_{GS}(J'', K)/hc. \quad (8)\end{aligned}$$

The parameters X^* are related to those in Eq. (1) as shown in Table I.

In Eq. (8), J' is given by $J'' + 1$ for the $\Delta J = +1$ transitions, by J'' for the $\Delta J = 0$ transitions, and by $J'' - 1$ for the $\Delta J = -1$ transitions; $l = +1$ for $\Delta K = +1$ and $l = -1$ for $\Delta K = -1$ transitions; E_{GS} is the ground state energy (J'' and K are the ground state rotational quantum numbers).

For $kl = +1$, $\Delta E_l^*(J', kl = +1)$ is

$$\Delta E_l^*(J', kl = +1)/hc = \pm 2[q_{22}^* + f_{22}^{(J)} J'(J'+1)]J'(J'+1), \quad (9)$$

where for $q_{22}^* > 0$, the lower sign holds for $\Delta J = 0$ transitions, and the upper sign holds for the $\Delta J = \pm 1$ transitions.

For $kl \neq +1$, we have

TABLE I

Determinable Combinations of Spectroscopic Parameters of the ν_6 Band[a]

Parameter X^*	ΣX_i	Parameter X^*	ΣX_i
$E_v^* \ (\equiv \nu_6^*)$	$E_v^0 + (A_6 - B_6) - 2(A\zeta^z)_6 - D_K + H_K + \eta_K + \tau_K + L_K + \sigma_K$	L_K^*	L_K
B_6^*	$B_6 - D_{JK} + H_{KJ} + \eta_J + \tau_{JK} + L_{KKJ} + \sigma_{KJ}$	η_J^*	$\eta_J - 2\,D_{JK} + 4\,H_{KJ} + 3\,\tau_{JK} + 6\,L_{KKJ} + 5\,\sigma_{KJ} - 2\,\Big((q_{22}^*)^2 +$
D_J^*	$D_J - H_{JK} - \tau_J - L_{JK} - \sigma_{JK}$		$+\, q_{22}^* f_{22}^{(J)} \Big) / \alpha$
D_{JK}^*	$D_{JK} - 6\,H_{KJ} - 3\,\tau_{JK} - 15\,L_{KKJ} - 10\,\sigma_{KJ}$	η_K^*	$\eta_K - 4\,D_K + 20\,H_K + 10\,\tau_K + 56\,L_K + 35\,\sigma_K + (q_{22}^*)^2/\,\alpha$
D_K^*	$D_K - 15\,H_K - 5\,\tau_K - 70\,L_K - 35\,\sigma_K$	τ_J^*	$\tau_J + 2\,H_{JK} + 4\,L_{JK} + 3\,\sigma_{JK} + 4\,\Big(q_{22}^* f_{22}^{(K)} - q_{22}^* f_{22}^{(J)} \Big) / \alpha$
H_J^*	$H_J + L_{JJK} + \sigma_J$	τ_{JK}^*	$\tau_{JK} + 4\,H_{KJ} + 20\,L_{KKJ} + 10\,\sigma_{KJ} - 2\,\Big(4\,q_{22}^* f_{22}^{(K)} - q_{22}^* f_{22}^{(J)} \Big) / \alpha$
H_{JK}^*	$H_{JK} + 6\,L_{JK} + 3\,\sigma_{JK}$	τ_K^*	$\tau_K + 6\,H_K + 56\,L_K + 21\,\sigma_K$
H_{KJ}^*	$H_{KJ} + 15\,L_{KKJ} + 5\,\sigma_{KJ}$	σ_J^*	$\sigma_J + 2\,L_{JJK}$
H_K^*	$H_K + 28\,L_K + 7\,\sigma_K$	σ_{JK}^*	$\sigma_{JK} + 4\,L_{JK}$
$(A_6 - B_6)^*$	$(A_6 - B_6) - 6\,D_K + 15\,H_K + 3\,\eta_K + 10\,\tau_K + 28\,L_K + 21\,\sigma_K$	σ_{KJ}^*	$\sigma_{KJ} + 6\,L_{KKJ}$
$2(A\zeta^z)_6^*$	$2(A\zeta^z)_6 - 2\,(A_6 - B_6) + 4\,D_K - 6\,H_K - 3\,\eta_K - 5\,\tau_K - 8\,L_K +$	σ_K^*	$\sigma_K + 8\,L_K$
	$+\, 7\,\sigma_K + (q_{22}^*)^2/\alpha$ [b]	q_{22}^*	$q_{22} + 2\,f_{22}^{(K)}$
L_J^*	L_J	$f_{22}^{(J)*}$	$f_{22}^{(J)}$
L_{JJK}^*	L_{JJK}	f_{24}^*	f_{24}
L_{JK}^*	L_{JK}	$f_{24}^{(J)*}$	$f_{24}^{(J)}$
L_{KKJ}^*	L_{KKJ}		

[a] $X^* = \sum_i X_i$. [b] $\alpha = A_6 - B_6 - (A\zeta^z)_6$.

$$\Delta E_l^*(J', kl \neq +1)/hc$$

$$= \pm[q_{22}^* + f_{22}^{(J)}J(J+1)]^2[J(J+1)]^2/[A_6 - B_6 - (A\zeta^z)_6]K, \quad (10)$$

where the upper sign holds for the $\Delta K = +1$ transitions and the lower sign holds for the $\Delta K = -1$ transitions.

The parameter $f_{22}^{(K)}$ is completely correlated with other spectroscopic parameters; we used therefore $f_{22}^{(K)} = 0$ [cf. Ref. (*8*)] in fitting the data. The values of q_{12} and $f_{12}^{(J)}$ were constrained to zero for the same reason. The parameter $f_{12}^{(K)}$ can in principle be determined but we found its value to be so small for the ν_6 band that it could not be determined from the available data.

On the other hand, the $\Delta l = \pm 2$, $\Delta k = \mp 4$ interaction leads to a measurable splitting of the $kl = -2$ levels in the ν_6 band of $^{12}CH_3F$ (Fig. 1), from which it was possible to determine $|f_{24}|$, $|f_{24}^{(J)}|$ and the relative sign of f_{24} and $f_{24}^{(J)}$ (Table III).

The $\Delta J = +1$, $\Delta K = 0$, $\Delta l = 0$ selection rules for the pure rotational transitions in the $v_6 = 1$ state give the following expression for the transition frequencies ν_{rot} in terms of the determinable parameters (given in cm^{-1}):

$$\begin{aligned}\nu_{\text{rot}}/c = 2B_6^*(J+1) + \{&-4D_J^*(J+1)^3 - 2D_{JK}^*(J+1)(Kl-1)^2 \\ &+ H_J^*(J+1)^3[(J+2)^3 - J^3] + 4H_{JK}^*(J+1)^3(Kl-1)^2 \\ &+ 2H_{KJ}^*(J+1)(Kl-l)^4 + \cdots\} + [2\eta_J^*(J+1)(Kl-1) \\ &+ 4\tau_J^*(J+1)^3(Kl-1) + 2\tau_{JK}^*(J+1)(Kl-1)^3 \cdots] + \Delta\nu, \quad (11)\end{aligned}$$

where the expression for $\Delta\nu$ depends on kl; for $kl = +1$, the diagonal contribution of the 2,2 l-type operator,

$$\Delta\nu_d = \pm 4[q_{22}^*(J+1) + 2f_{22}^{(J)}(J+1)^3], \quad (12)$$

gives a splitting of the rotational spectrum lines while for $kl \neq +1$, the off-diagonal effect of this interaction causes a shift of the line positions by

$$\Delta\nu_{\text{off-d}} = [|\Delta E_l^*(J+1, kl)| - |\Delta E_l^*(J, kl)|]/hc, \quad (13)$$

where ΔE_l^* is defined by Eq. (10).

For $kl = -2$, the diagonal contribution of the $\Delta l = \pm 2$, $\Delta k = \mp 4$ interaction gives

$$\Delta\nu_2 = \pm 4[2f_{24} + 3f_{24}^{(J)}(J+1)^2](J+1)(J+2). \quad (14)$$

IV. RESULTS

We have fitted separately the ground state (*9, 15–17*) and $v_6 = 1$ rotational transition frequencies (*17–20*), the rovibrational ν_6 line positions, and simultaneously all the rotational and rovibrational line positions. In each of these least-squares adjustments of the spectroscopic parameters, the results of which are given in Tables II and III, each transition was weighted by the inverse square of its experimental uncertainty. The uncertainty of the isolated and symmetric rovibrational line positions was estimated to be 3×10^{-5} cm^{-1}. The uncertainties of the rotational transition frequencies in the ground state were taken from Refs. (*9, 15–17*), those for the $v_6 = 1$ state are indicated in Table A2.

Calculated and experimental values of the ν_6 band rovibrational line positions are compared in Table A1. Parameters which are obtained by a transformation inverse to that which is given in Table I are given in Table IV. They were calculated from the values of the parameters given in column II of Table III. The spectroscopic parameters in Table III and the line positions given in Table A1 are the most precise physical quantities for the ν_6 band of $^{12}CH_3F$ which have been obtained so far. Up to $J \leqslant 20$, the smoothed values of the wavenumbers could be used as a suitable calibration standard with better than 10^{-4} cm^{-1} accuracy. There is, however, a point which requires further work, namely, the systematic differences of the order of magnitude 10^{-4} cm^{-1} between the calculated and observed wavenumbers which appear for $J > 20$ and have opposite signs for $\Delta K = +1$ and $\Delta K = -1$ transitions (see Tables A1 and A2). We have not been able to remove them by introducing some other higher-order terms in the fit. It seems that one should take into account explicitly the x–y Coriolis interaction between $v_3 = 1$ and $v_6 = 1$ vibrational levels in order to arrive at a quantitative fit of the data for the high J values. The x–y Coriolis interaction between the $v_6 = 1$ and $v_2 = 1$ vibrational levels ($v_2 = 1$ level interacts strongly also with the $v_5 = 1$ level) might also be expected to be responsible for this effect.

This neglected interaction is probably the reason why we have larger standard errors for the ground state parameters obtained by fitting our data for the ν_6 band than those

TABLE II

Ground State Parameters of $^{12}CH_3F$ (in MHz Units)

Parameter	I[a]	II[b]	III[c]	IV[d]
A	-	155 352.8	155 352.8	-
B	25 536.14965 (26)[e]	25 536.16198 (2144)	25 536.15010 (133)	25 536.1499 (6)
$D_J \times 10^3$	60.23184 (142)	60.23662 (2394)	61.22715 (576)	60.2330 (36)
$D_{JK} \times 10^3$	439.6000 (144)	440.6961 (1627)	439.6911 (661)	439.5743 (312)
$D_K \times 10^3$	-	2108.	2108.	-
$H_J \times 10^6$	-0.0210 (22)	-0.0275 (86)	-0.0301 (58)	-0.0218 (68)
$H_{JK} \times 10^6$	1.7765 (276)	2.5104 (11655)	1.8785 (940)	1.7518 (758)
$H_{KJ} \times 10^6$	21.7613 (862)	29.7281 (207302)	21.9731 (4228)	21.6679 (1921)

[a]Our fit to the ground state rotational transition frequencies taken from Refs. (9, 15-17). No. of data : 99, standard deviation of the fit : 0.016 MHz.

[b]Fit to the transition wavenumbers of the ν_6 band. The ground state parameters A and D_K were fixed to the values given by Graner (21).

[c]Simultaneous fit to all microwave, submillimeterwave, and ν_6 band transition line positions.

[d]From Ref. (9), fit to the $v_3 = 0$ and $v_3 = 1$ rotational and ν_3 band vib-rot line positions.

[e]Figures in parentheses are standard errors in units of the last digit quoted.

TABLE III

Parameters of the ν_6 Band of $^{12}CH_3F$ (in cm^{-1})

Parameter X^*	I[a]	II[b]	III[c]	Parameter X^*	I[a]	II[b]	III[c]
E_v^* ($\equiv \nu_6^*$)	1183.939966 (15)[d]	1183.939989 (12)	-	$\eta_K^* \times 10^6$	-219.202 (177)	-219.552 (128)	-
B_6^*	0.847904911 (750)	0.847904371 (114)	0.847903938 (265)	$\tau_J^* \times 10^9$	2.626 (119)	2.594 (100)	3.012 (227)
$D_J^* \times 10^6$	2.02400 (76)	2.02363 (25)	2.01529 (355)	$\tau_{JK}^* \times 10^9$	15.781 (800)	18.474 (511)	19.387 (567)
$D_{JK}^* \times 10^6$	15.39635 (5922)	15.31957 (939)	15.31404 (128)	$\tau_K^* \times 10^9$	-9.85 (185)	-10.17 (112)	-
$D_K^* \times 10^6$	72.6734 (354)	72.4870 (251)	-	$\sigma_J^* \times 10^{13}$	-3.034 (838)	-2.228 (732)	-
$H_J^* \times 10^{10}$	-	-	-0.280 (141)	$\sigma_{JK}^* \times 10^{13}$	178.18 (1127)	145.21 (722)	-
$H_{JK}^* \times 10^{10}$	-0.704 (503)	-1.222 (218)	-1.482 (503)	$q_{22}^* \times 10^6$	-73.1553 (535)	-73.1603 (481)	-73.5081 (1811)
$H_{KJ}^* \times 10^{10}$	14.755 (7675)	1.641 (935)	-	$f_{22}^{(J)} \times 10^8$	1.80727 (715)	1.80820 (637)	1.92007 (9005)
$\Delta H_K^* \times 10^{10}$	10.367 (2106)	0.866 (1734)	-	$f_{24}^* \times 10^{10}$	-70.370 (1936)	-70.370 (1867)	-
$(A_6 - B_6)^*$	4.35002452 (164)	4.35001746 (123)	-	$f_{24}^{(J)} \times 10^{13}$	4.98 (233)	4.98 (224)	-
$2(A\zeta^z)_6^*$	-5.61575815 (510)	-5.61576225 (424)	-				
$L_{JJK}^* \times 10^{12}$	0.0496 (178)	0.0408 (145)					
$L_{JK}^* \times 10^{12}$	-1.968 (191)	-1.289 (118)					
$L_{KKJ}^* \times 10^{12}$	-3.948 (655)	0.286 (431)					
$\eta_J^* \times 10^6$	5.6225 (483)	5.6013 (385)	5.5667 (485)				

Type of data	I No. Data	I St.dev.	II No. Data	II St.dev.	III No. Data	III St.dev.
Ground st. rot.	-	-	99	0.02 MHz	-	-
Upper st. rot.	-	-	135	0.47 MHz	135	0.30 MHz
Vib - rot	1070	3.58 MHz	1070	3.70 MHz	-	-

[a] Fit to our FTS line positions of the ν_6 band. The ground state parameters A_0 and D_K^0 were fixed to the values given by Graner (21) (see Table II).

[b] Simultaneous fit to the rovibrational wavenumbers, ground and $v_6 = 1$ state rotational transition frequencies.

[c] Fit to the upper state pure rotational frequencies [cf. Ref. (20)].

[d] Figures in parentheses are standard errors in units of the last digit quoted.

obtained by Lee *et al.* (*9*) from the ν_3 band of $^{12}CH_3F$ (Table II). We could, of course, improve the ground state parameters by using combination differences from the ν_6 band. However, we have remeasured with Doppler-limited resolution the ν_3 band and the ν_2, ν_5 bands of $^{12}CH_3F$, where we have been able to assign a number of forbidden vibration–rotation transitions. Furthermore, we have measured more than 200 pure rotational transitions in the $v_2 = 1$ and $v_5 = 1$ vibrational states (*22*).

We plan to process simultaneously all these data taking into account various rovibrational interactions using a variational approach, which should lead to precise ground state as well as the ν_3, ν_6, ν_2, and ν_5 parameters.

The fact that an effective Hamiltonian describes experimental data less precisely for higher values of J is of course related to its theoretical accuracy. Badaqui and Champion (*23*) have proposed to weight data in merged fits such that the weights reflect not only the experimental precision $\Delta\sigma_i$ but also the theoretical accuracy of the model $\{w_i(J) = [(\Delta\sigma_i)^2 + \alpha^2 J^8]^{-1}\}$. There is no doubt that this approach leads to "less effective" and more consistent parameters. When we applied this approach to our data, we arrived at slightly better deviations for the infrared and submillimeter-wave data but the differences $|\nu_i(\exp) - \nu_i(\text{calc})|$ were an order of magnitude larger for $J > 20$. For reasons described above and because primarily we wished to provide reliable experimental data rather than the final values of spectroscopic parameters in this paper, we have decided to present our data using standard weights $w_i(J) = (\Delta\sigma_i)^{-2}$.

TABLE IV

Parameters of the ν_6 Band of $^{12}CH_3F$ (in cm^{-1}) Taken from Table III

Parameter	This work	Ref. (3)	Parameter	This work	Ref. (3)
ν_6	1182.674392 (17)[a]	1182.67605[b] (18)	$L_{JK} \times 10^{12}$	-1.289 (118)	-
B_6	0.847883432 (162)	0.847884295 (480)	$L_{KKJ} \times 10^{12}$	0.29 (43)	-
$D_J \times 10^6$	2.026360 (369)	2.0552 (1398)	$\eta_J \times 10^6$	36.2953 (592)	38.2398 (1514)
$D_{JK} \times 10^6$	15.37401 (1149)	15.2522 (1409)	$\eta_K \times 10^6$	70.2924 (2436)	-320.2[a] (220)
$D_K \times 10^6$	72.43491 (3332)	70.315[b]	$\tau_J \times 10^9$	2.887 (146)	
$H_J \times 10^{10}$	0.0026 (9)	-1.222 (218)	$\tau_{JK} \times 10^9$	17.812 (894)	
$H_{JK} \times 10^{10}$	-1.580 (247)	2.412 (2932)	$\tau_K \times 10^9$	-10.688 (2157)	
$H_{KJ} \times 10^{10}$	1.684 (999)	-53.470 (11498)	$\sigma_J \times 10^{12}$	-0.3044 (1022)	
$\Delta H_K \times 10^{10}$	0.866 (1734)	-	$\sigma_{JK} \times 10^{12}$	19.677 (1196)	
$(A_6 - B_6)$	4.35024130 (178)	4.352715[b] (1400)	$\sigma_{KJ} \times 10^{12}$	-1.717 (2588)	
$2(A\zeta^z)_6$	3.08464144 (622)	3.0874[b] (22)	$q_{22} \times 10^6$	-73.1603 (481)	72.720 (330)
$L_{JJK} \times 10^{12}$	0.0408 (145)	-	$f_{22}^{(J)} \times 10^8$	1.80820 (637)	-1.7910 (215)

[a] Figures in parentheses are standard errors in units of the last digit quoted.

[b] Constrained to the value given in Ref. (2); figures in parentheses are errors indicated in Ref. (2).

APPENDIX

TABLE A1

Assignment of Observed Transitions in the ν_6 Band of $^{12}CH_3F$ (in cm^{-1})

Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc
1	pP(21,13)	1077.345930 (-)*	-3263	51	pP(32, 6)	1092.827336 (-)*	-200	101	pP(23, 7)	1104.598171 (200)	233	151	pP(12, 9)	1114.217201 (30)	-79	201	pP(27, 2)	1124.203137 (30)	-271
2	pP(23,12)	1078.648981 (200)	12	52	pP(18,11)	1093.017629 (200)	-380	102	pP(20, 8)	1104.891218 (30)	108	152	pP(32, 2)	1114.649382 (200)	-416	202	pP(24, 3)	1124.336323 (1000)	-216
3	pP(31, 9)	1078.862186 (200)	-711	53	pP(29, 7)	1093.250445 (200)	92	103	pP(17, 9)	1105.171447 (100)	150	153	pP(29, 3)	1114.874448 (100)	-283	203	pP(24, 3)	1124.344569 (1000)	-182
4	pP(20,13)	1079.204932 (-)*	-2533	54	pP(15,12)	1093.410894 (30)	97	104	pP(34, 3)	1105.243842 (200)	-494	154	pP(29, 3)	1114.891914 (100)	-268	204	pP(21, 4)	1124.462902 (30)	-130
5	pP(25,11)	1079.969646 (-)*	-5777	55	pP(26, 8)	1093.665352 (200)	48	105	pP(34, 3)	1105.276519 (200)	-383	155	pP(26, 4)	1115.104710 (30)	-252	205	pP(18, 5)	1124.569837 (30)	-69
6	pP(22,12)	1080.521215 (200)	-127	56	pP(23, 9)	1094.071378 (100)	91	106	pP(14,10)	1105.437213 (30)	106	156	pP(23, 5)	1115.313615 (30)	-133	206	pP(15, 6)	1124.660411 (30)	-10
7	pP(30, 9)	1080.788388 (200)	-817	57	pP(34, 5)	1094.343738 (1000)	-470	107	pP(31, 4)	1105.576626 (200)	-506	157	pP(20, 6)	1115.509021 (30)	-38	207	pP(12, 7)	1124.733507 (30)	-53
8	pP(19,13)	1081.056811 (2000)	-999	58	pP(20,10)	1094.467096 (-)*	123	108	pP(11,11)	1105.686822 (200)	-149	158	pP(17, 7)	1115.689992 (30)	31	208	pP(9, 8)	1124.788033 (30)	-91
9	pP(27,10)	1081.326925 (1000)	-1662	59	pP(31, 6)	1094.755364 (100)	-117	109	pP(28, 5)	1105.883435 (100)	-318	159	pP(14, 8)	1115.855362 (30)	17	209	rP(32, 0)	1125.926158 (30)	160
10	pP(24,11)	1081.857037 (330)	-4382	60	pP(17,11)	1094.850719 (500)	-101	110	pP(25, 6)	1106.179761 (30)	-67	160	pP(11, 9)	1116.003850 (30)	-74	210	pP(29, 1)	1125.961624 (100)	-173
11	pP(32, 8)	1082.183125 (200)	79	61	pP(28, 7)	1095.159423 (200)	310	111	pP(22, 7)	1106.464552 (30)	34	161	pP(34, 1)	1116.346251 (-)*	-129	211	pP(26, 2)	1126.094083 (30)	-233
12	pP(21,12)	1082.385885 (200)	-71	62	pP(14,12)	1095.221336 (100)	226	112	pP(19, 8)	1106.736861 (30)	66	162	pP(31, 2)	1116.572989 (200)	-610	212	pP(23, 3)	1126.208103 (5000)	-228
13	pP(29, 9)	1082.707881 (5000)	-449	63	pP(22, 9)	1095.939737 (100)	81	113	pP(16, 9)	1106.995504 (30)	64	163	pP(28, 3)	1116.780434 (30)	-269	213	pP(23, 3)	1126.215013 (5000)	-240
14	pP(18,13)	1082.900007 (2000)	-232	64	pP(33, 5)	1096.283728 (200)	-393	114	pP(33, 3)	1107.183233 (200)	-484	164	pP(28, 3)	1116.795543 (30)	-347	214	pP(20, 4)	1126.313792 (30)	-88
15	pP(26,10)	1083.226394 (330)	-1362	65	pP(19,10)	1096.314021 (200)	-79	115	pP(33, 3)	1107.212169 (200)	-539	165	pP(25, 4)	1116.990018 (30)	-282	215	pP(17, 5)	1126.399846 (30)	-54
16	pP(34, 7)	1083.603538 (200)	472	66	pP(16,11)	1096.676400 (500)	398	116	pP(13,10)	1107.238984 (30)	-68	166	pP(22, 5)	1117.178831 (30)	-192	216	pP(14, 6)	1126.468993 (30)	6
17	pP(31, 8)	1084.114463 (200)	105	67	pP(30, 6)	1096.676400 (500)	-252	117	pP(30, 4)	1107.495580 (200)	-485	167	pP(19, 6)	1117.353711 (30)	21	217	pP(11, 7)	1126.520175 (30)	70
18	pP(20,12)	1084.242958 (30)	143	68	pP(13,12)	1097.021227 (-)*	-2417	118	pP(27, 5)	1107.783269 (30)	-188	168	pP(16, 7)	1117.513328 (30)	-24	218	pP(8, 8)	1126.551943 (30)	-92
19	pP(28, 9)	1084.619983 (200)	-271	69	pP(27, 7)	1097.060926 (-)*	15	119	pP(24, 6)	1108.059648 (30)	-65	169	pP(13, 8)	1117.656873 (30)	-12	219	rP(34, 1)	1127.598967 (200)	447
20	pP(17,13)	1084.734698 (2000)	-61	70	pP(24, 8)	1097.436191 (100)	215	120	pP(21, 7)	1108.323926 (30)	-47	170	pP(10, 9)	1117.782878 (30)	-105	220	rP(31, 0)	1127.843699 (30)	78
21	pP(25,10)	1085.118561 (200)	-963	71	pP(21, 9)	1097.800536 (30)	-168	121	pP(18, 8)	1108.575235 (30)	44	171	pP(33, 1)	1118.282210 (200)	-88	221	pP(28, 1)	1127.865292 (30)	-133
22	pP(33, 7)	1085.546065 (200)	-164	72	pP(18,10)	1098.153900 (30)	158	122	pP(15, 9)	1108.812221 (30)	86	172	pP(30, 2)	1118.490606 (100)	-294	222	pP(25, 2)	1127.978311 (30)	-218
23	pP(22,11)	1085.608329 (200)	-2331	73	pP(32, 5)	1098.216980 (200)	-437	123	pP(12,10)	1109.033266 (30)	-128	173	pP(27, 3)	1118.679523 (30)	-377	223	pP(22, 3)	1128.073077 (5000)	-117
24	pP(30, 8)	1086.038816 (200)	157	74	pP(15,11)	1098.493451 (-)*	-91	124	pP(32, 3)	1109.116140 (80)	-338	174	pP(27, 3)	1118.692796 (30)	-250	224	pP(22, 3)	1128.078846 (5000)	-134
25	pP(19,12)	1086.092152 (200)	232	75	pP(29, 6)	1098.590800 (100)	-219	125	pP(32, 3)	1109.141773 (100)	-410	175	pP(24, 4)	1118.868589 (30)	-222	225	pP(19, 4)	1128.157623 (30)	-98
26	pP(27, 9)	1086.524721 (330)	-241	76	pP(12,12)	1098.818295 (30)	-93	126	pP(29, 4)	1109.408022 (100)	-328	176	pP(21, 5)	1119.037201 (30)	-109	226	pP(16, 5)	1128.222726 (30)	-5
27	pP(16,13)	1086.561729 (1000)	352	77	pP(26, 7)	1098.955707 (200)	-12	127	pP(26, 5)	1109.676065 (30)	-277	177	pP(18, 6)	1119.191141 (30)	-34	227	pP(13, 6)	1128.270250 (30)	15
28	pP(21,11)	1087.472233 (-)*	-1664	78	pP(23, 8)	1099.310655 (100)	84	128	pP(23, 6)	1109.932563 (30)	-46	178	pP(15, 7)	1119.329432 (30)	-9	228	pP(10, 7)	1128.299200 (30)	23
29	pP(32, 7)	1087.482894 (330)	326	79	pP(20, 9)	1099.654545 (30)	132	129	pP(20, 7)	1110.176345 (30)	72	179	pP(12, 8)	1119.450884 (30)	-81	229	rP(33, 1)	1129.533407 (200)	541
30	pP(18,12)	1087.933458 (1000)	185	80	pP(34, 4)	1099.780271 (300)	-540	130	pP(17, 8)	1110.406290 (30)	19	180	pP(9, 9)	1119.554232 (30)	-193	230	rP(30, 0)	1129.754763 (5000)	49
31	pP(29, 8)	1087.956296 (1000)	369	81	pP(17,10)	1099.985977 (30)	96	131	pP(14, 9)	1110.621339 (30)	-19	181	pP(32, 1)	1120.211575 (100)	-265	231	pP(27, 1)	1129.762424 (5000)	-48
32	pP(15,13)	1088.380506 (200)	410	82	pP(31, 5)	1100.143609 (200)	-453	132	pP(34, 2)	1110.782202 (200)	-652	182	pP(29, 2)	1120.401259 (40)	-402	232	pP(24, 2)	1129.855774 (30)	-232
33	pP(26, 9)	1088.422356 (80)	-80	83	pP(14,11)	1100.303508 (100)	82	133	pP(11,10)	1110.819984 (30)	-126	183	pP(26, 3)	1120.572021 (100)	-272	233	pP(21, 3)	1129.930979 (-)*	-116
34	pP(23,10)	1088.881109 (1000)	294	84	pP(28, 6)	1100.498516 (30)	-35	134	pP(31, 3)	1111.042071 (80)	-517	184	pP(26, 3)	1120.583341 (100)	-263	234	pP(21, 3)	1129.935672 (-)*	-218
35	pP(34, 6)	1088.951301 (830)	-149	85	pP(25, 7)	1100.843645 (100)	134	135	pP(31, 3)	1111.064899 (80)	-385	185	pP(23, 4)	1120.740301 (30)	-160	235	pP(18, 4)	1129.994494 (30)	-24
36	pP(20,11)	1089.328481 (1000)	-1057	86	pP(22, 8)	1101.178158 (100)	184	136	pP(28, 4)	1111.313639 (30)	-312	186	pP(20, 5)	1120.888489 (30)	-87	236	pP(15, 5)	1130.038326 (30)	-38
37	pP(31, 7)	1089.412093 (200)	40	87	pP(19, 9)	1101.500854 (30)	93	137	pP(25, 5)	1111.562206 (30)	-168	187	pP(17, 6)	1121.021502 (30)	21	237	pP(12, 6)	1130.064154 (-)*	24
38	pP(17,12)	1089.767187 (1000)	314	88	pP(33, 4)	1101.719097 (200)	-372	138	pP(22, 6)	1111.798428 (30)	-59	188	pP(14, 7)	1121.138159 (30)	-34	238	pP(9, 7)	1130.064154 (-)*	-6586
39	pP(28, 8)	1089.866296 (200)	158	89	pP(16,10)	1101.810544 (30)	43	139	pP(19, 7)	1112.021386 (30)	-5	189	pP(11, 8)	1121.237537 (30)	-17	239	rP(32, 1)	1131.461304 (200)	394
40	pP(14,13)	1090.191060 (200)	143	90	pP(30, 5)	1102.063598 (200)	-424	140	pP(16, 8)	1112.230086 (30)	78	190	pP(31, 1)	1122.134726 (-)*	-238	240	pP(26, 1)	1131.652815 (5000)	-83
41	pP(25, 9)	1090.312741 (40)	81	91	pP(13,11)	1102.105423 (200)	-215	141	pP(13, 9)	1112.423005 (30)	-77	191	pP(28, 2)	1122.305494 (30)	-349	241	rP(29, 0)	1131.659397 (5000)	136
42	pP(22,10)	1090.749528 (200)	-789	92	pP(27, 6)	1102.399146 (30)	-70	142	pP(10,10)	1112.598919 (30)	-253	192	pP(25, 3)	1122.457625 (100)	-224	242	pP(23, 2)	1131.726512 (30)	-197
43	pP(33, 6)	1090.892785 (200)	-63	93	pP(24, 7)	1102.724252 (-)*	-8	143	pP(33, 2)	1112.719099 (200)	-438	193	pP(25, 3)	1122.467267 (100)	-253	243	pP(20, 3)	1131.781878 (-)*	-124
44	pP(19,11)	1091.177016 (200)	-562	94	pP(21, 8)	1103.038249 (30)	87	144	pP(30, 3)	1112.961560 (100)	-456	194	pP(22, 4)	1122.605000 (30)	-214	244	pP(20, 3)	1131.785660 (-)*	-277
45	pP(30, 7)	1091.334752 (200)	95	95	pP(18, 9)	1103.339861 (30)	131	145	pP(30, 3)	1112.981468 (80)	-497	195	pP(19, 5)	1122.732718 (30)	-69	245	pP(17, 4)	1131.824161 (30)	-72
46	pP(16,12)	1091.593085 (100)	369	96	pP(15,10)	1103.627600 (30)	17	146	pP(27, 4)	1113.212497 (30)	-337	196	pP(16, 6)	1122.844546 (30)	-29	246	pP(8, 7)	1131.834700 (200)	-56
47	pP(27, 8)	1091.769359 (-)*	88	97	pP(32, 4)	1103.651016 (200)	-573	147	pP(24, 5)	1113.441373 (30)	-148	197	pP(13, 7)	1122.939544 (30)	-34	247	pP(14, 5)	1131.846833 (-)*	71
48	pP(13,13)	1091.991808 (-)*	-2031	98	pP(12,11)	1103.900096 (200)	-64	148	pP(21, 6)	1113.657297 (30)	-17	198	pP(10, 8)	1123.016505 (30)	-114	248	pP(11, 6)	1131.850545 (-)*	-91
49	pP(24, 9)	1092.195658 (100)	42	99	pP(29, 5)	1103.976941 (100)	-323	149	pP(18, 7)	1113.859317 (30)	20	199	rP(33, 0)	1124.002275 (200)	416	249	pQ(21, 9)	1133.281653 (2000)	489
50	pP(21,10)	1092.612323 (-)*	-51	100	pP(26, 6)	1104.292930 (30)	-56	150	pP(15, 8)	1114.046381 (30)	5	200	pP(30, 1)	1124.051513 (100)	-117	250	rP(34, 2)	1133.281653 (2000)	445

TABLE A1—*Continued*

Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc
251	rP(31, 1)	1133.382885 (100)	274	301	pP(19, 2)	1139.140863 (-)*	-126	351	rP(22, 0)	1144.806339 (30)	-11	401	rP(22, 1)	1150.385616 (1000)	49	451	pQ(13, 5)	1155.664744 (30)	33
252	pQ(20, 9)	1133.452054 (200)	-60	302	pP(22, 1)	1139.147465 (-)*	-116	352	pQ(14, 7)	1144.834635 (30)	-43	402	rP(25, 2)	1150.456027 (30)	218	452	pQ(12, 5)	1155.767354 (30)	-19
253	pP(25, 1)	1133.536566 (30)	-97	303	pQ(17, 8)	1139.159673 (-)*	355	353	pQ(13, 7)	1144.946630 (200)	290	403	pQ(11, 6)	1150.480679 (30)	7	453	rP(16, 0)	1155.814187 (30)	69
254	rP(28, 0)	1133.557239 (30)	-8	304	rP(25, 0)	1139.211608 (30)	-51	354	pQ(12, 7)	1145.049891 (30)	-69	404	rP(28, 3)	1150.506683 (30)	266	454	pQ(11, 5)	1155.862141 (30)	43
255	pP(22, 2)	1133.590799 (1000)	200	305	pQ(16, 8)	1139.296320 (-)*	266	355	pQ(11, 7)	1145.145494 (30)	-57	405	rP(31, 4)	1150.537911 (-)*	320	455	rP(19, 1)	1155.933041 (30)	65
256	pP(7, 7)	1133.590799 (1000)	-387	306	pQ(15, 8)	1139.424776 (100)	147	356	pQ(10, 7)	1145.233372 (200)	245	406	pQ(10, 6)	1150.567813 (30)	-17	456	pQ(10, 5)	1155.948964 (30)	70
257	pQ(19, 9)	1133.615059 (-)*	346	307	pQ(14, 8)	1139.545040 (100)	-23	357	pQ(9, 7)	1145.312600 (30)	-101	407	pQ(9, 6)	1150.646987 (30)	-44	457	pQ(9, 5)	1156.027792 (30)	21
258	pP(19, 3)	1133.629467 (-)*	3584	308	pQ(13, 8)	1139.657435 (100)	58	358	pQ(8, 7)	1145.384296 (200)	13	408	pQ(8, 6)	1150.718215 (30)	-68	458	rP(22, 2)	1156.063230 (30)	113
259	pP(19, 3)	1133.629467 (-)*	390	309	pQ(12, 8)	1139.761658 (100)	71	359	pP(6, 5)	1146.048818 (30)	-16	409	pQ(7, 6)	1150.781537 (30)	-59	459	pQ(8, 5)	1156.098693 (30)	-44
260	pP(10, 6)	1133.629467 (-)*	-246	310	pQ(11, 8)	1139.857883 (100)	171	360	pP(9, 4)	1146.202379 (30)	7	410	pQ(6, 6)	1150.836899 (30)	-79	460	pQ(7, 5)	1156.161817 (30)	18
261	pP(16, 4)	1133.647392 (-)*	563	311	pQ(10, 8)	1139.945733 (100)	-36	361	pP(12, 3)	1146.333727 (1000)	264	411	pP(6, 4)	1151.472557 (30)	-5	461	rP(25, 3)	1156.172265 (30)	176
262	pP(13, 5)	1133.647392 (1000)	-495	312	pP(6, 6)	1140.670945 (30)	-17	362	pP(12, 3)	1146.333727 (1000)	-214	412	pP(9, 3)	1151.670750 (100)	79	462	pQ(6, 5)	1156.216967 (30)	3
263	pQ(18, 9)	1133.769481 (1000)	491	313	pP(9, 5)	1140.778890 (30)	4	363	pP(15, 2)	1146.443664 (30)	-35	413	pP(9, 3)	1151.670753 (100)	-60	463	rP(28, 4)	1156.260570 (-)*	467
264	pQ(17, 9)	1133.915113 (200)	141	314	pP(12, 4)	1140.865235 (30)	-13	364	pP(18, 1)	1146.533045 (30)	-28	414	pP(12, 2)	1151.845889 (30)	-54	464	pQ(5, 5)	1156.264201 (-)*	-36
265	pQ(16, 9)	1134.052955 (-)*	270	315	pP(15, 3)	1140.931090 (-)*	615	365	rP(24, 1)	1146.653539 (-)*	144	415	pP(15, 1)	1151.998925 (30)	-26	465	rP(31, 5)	1156.327354 (-)*	59
266	pQ(15, 9)	1134.182245 (100)	88	316	pP(15, 3)	1140.931093 (-)*	-594	366	rP(21, 0)	1146.657847 (-)*	-28	416	rP(18, 0)	1152.172065 (30)	62	466	pP(6, 3)	1156.941095 (30)	53
267	pQ(14, 9)	1134.303391 (100)	-20	317	rP(33, 3)	1140.931093 (-)*	-3805	367	rP(27, 2)	1146.684665 (500)	224	417	rP(21, 1)	1152.241581 (30)	55	467	pP(6, 3)	1156.941095 (30)	30
268	pQ(13, 9)	1134.416154 (100)	-316	318	pP(18, 2)	1140.977307 (2000)	79	368	rP(30, 3)	1146.697285 (500)	389	418	rP(24, 2)	1152.331718 (30)	130	468	pP(9, 2)	1157.182830 (30)	6
269	pQ(12, 9)	1134.521528 (200)	170	319	rP(30, 2)	1140.977307 (2000)	-1209	369	pQ(29, 6)	1147.535381 (-)*	-435	419	rP(27, 3)	1152.401770 (30)	270	469	pP(12, 1)	1157.400825 (30)	30
270	pQ(11, 9)	1134.618075 (200)	-19	320	pP(21, 1)	1141.004554 (2000)	261	370	pQ(28, 6)	1147.768340 (200)	-289	420	rP(30, 4)	1152.451899 (-)*	433	470	rP(15, 0)	1157.624974 (100)	73
271	rP(33, 2)	1135.215664 (200)	679	321	rP(27, 1)	1141.004554 (2000)	-593	371	pP(5, 5)	1147.790388 (30)	42	421	pQ(28, 5)	1153.163479 (-)*	-656	471	rP(18, 1)	1157.768401 (30)	22
272	rP(30, 1)	1135.298261 (100)	334	322	rP(24, 0)	1141.083207 (30)	-13	372	pP(8, 4)	1147.966665 (30)	57	422	pP(5, 4)	1153.214199 (30)	-7	472	rP(21, 2)	1157.918940 (30)	160
273	pP(9, 6)	1135.401373 (30)	48	323	pP(8, 5)	1142.543067 (30)	6	373	pP(11, 3)	1148.120100 (1000)	208	423	pQ(27, 5)	1153.386796 (-)*	-560	473	rP(24, 3)	1158.047715 (30)	210
274	pP(24, 1)	1135.413682 (100)	-43	324	pP(11, 4)	1142.651697 (200)	33	374	pP(11, 3)	1148.120100 (1000)0	-124	424	pP(8, 3)	1153.434988 (30)	46	474	rP(27, 4)	1158.154982 (200)	210
275	pP(12, 5)	1135.441727 (-)*	27	325	pP(14, 3)	1142.739140 (2000)	423	375	pQ(26, 6)	1148.209542 (30)	-27	425	pP(8, 3)	1153.434988 (30)	-39	475	rP(30, 5)	1158.240894 (-)*	181
276	pP(21, 2)	1135.448063 (-)*	428	326	pP(14, 3)	1142.739142 (2000)	-485	376	pP(14, 2)	1148.251629 (30)	-10	426	pQ(26, 5)	1153.602418 (100)	-22	476	pQ(29, 4)	1158.371959 (-)*	-688
277	rP(27, 0)	1135.448063 (-)*	-591	327	pP(17, 2)	1142.806358 (30)	-94	377	pP(17, 1)	1148.362000 (30)	-77	427	pP(11, 2)	1153.632160 (30)	-63	477	pQ(28, 4)	1158.602513 (-)*	-293
278	pP(18, 3)	1135.462670 (-)*	-35	328	pP(20, 1)	1142.854096 (200)	-44	378	pQ(25, 6)	1148.417639 (100)	-92	428	pP(14, 1)	1153.806758 (30)	21	478	pP(5, 3)	1158.682850 (30)	64
279	pP(15, 4)	1135.462674 (-)*	406	329	rP(32, 3)	1142.862160 (1000)	293	379	rP(20, 0)	1148.502703 (30)	27	429	pQ(25, 5)	1153.806758 (-)*	-2644	479	pP(5, 3)	1158.682852 (30)	56
280	pP(18, 3)	1135.462674 (-)*	-2593	330	rP(29, 2)	1142.887131 (-)*	182	380	rP(23, 1)	1148.522926 (30)	84	430	rP(17, 0)	1153.996544 (30)	68	480	pQ(27, 4)	1158.824506 (200)	-375
281	rP(32, 2)	1137.142876 (200)	385	331	rP(26, 1)	1142.894620 (-)*	115	381	rP(26, 2)	1148.573644 (100)	232	431	pQ(24, 5)	1154.008093 (200)	-164	481	pP(8, 2)	1158.947057 (30)	-0
282	pP(8, 6)	1137.165462 (30)	32	332	rP(23, 0)	1142.948128 (30)	5	382	rP(29, 3)	1148.605285 (100)	418	432	rP(20, 1)	1154.090761 (30)	84	482	pQ(26, 4)	1159.038522 (-)*	-364
283	rP(29, 1)	1137.207049 (100)	233	333	pQ(23, 7)	1143.465053 (200)	44	383	pQ(24, 6)	1148.617661 (30)	-51	433	rP(23, 2)	1154.200657 (-)*	-48	483	pP(11, 1)	1159.186918 (30)	-63
284	pP(11, 5)	1137.228214 (30)	49	334	pQ(22, 7)	1143.650016 (200)	180	384	pQ(23, 6)	1148.809422 (30)	-107	434	rP(26, 3)	1154.290337 (30)	265	484	pQ(25, 4)	1159.244578 (30)	-254
285	pP(14, 4)	1137.270474 (40)	-36	335	pQ(21, 7)	1143.826549 (200)	92	385	pQ(22, 6)	1148.993169 (30)	-32	435	rP(29, 4)	1154.359191 (200)	206	485	rP(14, 0)	1159.428842 (30)	50
286	pP(23, 1)	1137.283895 (-)*	-150	336	pQ(20, 7)	1143.994951 (200)	59	386	pQ(21, 6)	1149.168616 (30)	-128	436	pQ(22, 5)	1154.381672 (30)	-33	486	pQ(24, 4)	1159.442473 (30)	-260
287	pP(17, 3)	1137.293496 (-)*	1062	337	pQ(19, 7)	1144.155087 (200)	-73	387	pQ(20, 6)	1149.336106 (30)	-71	437	rP(32, 5)	1154.407682 (-)*	96	487	rP(17, 1)	1159.596868 (30)	26
288	pP(17, 3)	1137.293496 (-)*	-966	338	pP(7, 5)	1144.299779 (100)	54	388	pQ(19, 6)	1149.495396 (30)	-118	438	pQ(21, 5)	1154.556208 (30)	-120	488	pQ(23, 4)	1159.632419 (30)	-183
289	pP(20, 2)	1137.297357 (-)*	-422	339	pQ(18, 7)	1144.307139 (-)*	-144	389	pQ(18, 6)	1149.646724 (30)	-50	439	pQ(20, 5)	1154.722836 (30)	-67	489	rP(20, 2)	1159.767752 (30)	103
290	rP(26, 0)	1137.333388 (30)	-76	340	pP(10, 4)	1144.430729 (30)	5	390	pP(7, 4)	1149.723339 (30)	-9	440	pQ(19, 5)	1154.881286 (30)	-157	490	pQ(22, 4)	1159.814320 (30)	-130
291	pQ(20, 8)	1138.700450 (-)*	522	341	pQ(17, 7)	1144.451211 (100)	-66	391	pQ(17, 6)	1149.790033 (30)	61	441	pP(4, 4)	1154.948270 (30)	34	491	rP(23, 3)	1159.916459 (30)	182
292	pP(7, 6)	1138.922006 (30)	16	342	pP(13, 3)	1144.540058 (1000)	333	392	pP(10, 3)	1149.899139 (30)	164	442	pQ(18, 5)	1155.031850 (30)	114	492	pQ(21, 4)	1159.988121 (30)	-170
293	rP(34, 3)	1139.002256 (-)*	569	343	pP(13, 3)	1144.540058 (1000)	-336	393	pP(10, 3)	1149.899139 (30)	-57	443	pQ(17, 5)	1155.174337 (30)	140	493	rP(26, 4)	1160.043183 (100)	236
294	pP(10, 5)	1139.007248 (-)*	8	344	pQ(16, 7)	1144.587194 (200)	31	394	pQ(16, 6)	1149.925116 (30)	-7	444	pP(7, 3)	1155.191790 (30)	44	494	rP(29, 5)	1160.147942 (-)*	149
295	pQ(18, 8)	1139.014666 (-)*	266	345	pP(16, 2)	1144.628581 (30)	-42	395	pP(13, 2)	1150.052370 (30)	-31	445	pP(7, 3)	1155.191794 (30)	1	495	pQ(20, 4)	1160.154028 (30)	-109
296	rP(31, 2)	1139.063985 (-)*	303	346	pP(19, 1)	1144.697043 (30)	-37	396	pQ(14, 6)	1150.171326 (30)	-17	446	pQ(16, 5)	1155.308952 (30)	-44	496	rP(32, 6)	1160.230796 (500)	-28
297	pP(13, 4)	1139.071496 (-)*	-20	347	pQ(15, 7)	1144.715121 (200)	163	397	pP(16, 1)	1150.184009 (30)	-42	447	pP(10, 2)	1155.411214 (30)	16	497	pQ(19, 4)	1160.311877 (30)	-121
298	rP(28, 1)	1139.109615 ( )*	378	348	rP(25, 1)	1144.777366 (-)*	97	398	pQ(13, 6)	1150.282419 (30)	-21	448	pQ(15, 5)	1155.435534 (30)	0	498	pP(4, 3)	1160.416967 (30)	31
299	pP(16, 3)	1139.115840 (-)*	804	349	rP(31, 3)	1144.782901 ( )*	353	399	rP(19, 0)	1150.340771 (30)	-4	449	pQ(14, 5)	1155.554089 (30)	-13	499	pP(4, 3)	1160.416967 (30)	28
300	pP(16, 3)	1139.115840 (-)*	-776	350	rP(28, 2)	1144.789162 (-)*	223	400	pQ(12, 6)	1150.385616 (1000)	70	450	pP(13, 1)	1155.607374 (30)	8	500	pQ(18, 4)	1160.461731 (30)	-157

TABLE A1—*Continued*

Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc
501	pQ(17, 4)	1160.603722 (30)	-96	551	pQ(23, 3)	1165.105075 (200)	-152	601	pQ(3, 3)	1167.229796 (30)	76	651	pQ(6, 2)	1172.625393 (30)	-4	701	pQ(14, 1)	1177.525192 (30)	-23
502	pP(7, 2)	1160.703861 (30)	7	552	pQ(23, 3)	1165.113199 (200)	-240	602	pQ(3, 3)	1167.229796 (30)	72	652	pQ(5, 2)	1172.672241 (30)	-21	702	pQ(13, 1)	1177.634492 (30)	-22
503	pQ(16, 4)	1160.737713 (30)	-85	553	rP(17, 2)	1165.273069 (30)	17	603	rP(19, 3)	1167.324104 (30)	93	653	pQ(4, 2)	1172.711252 (30)	-60	703	pQ(12, 1)	1177.735941 (30)	-39
504	pQ(15, 4)	1160.863734 (30)	-104	554	pQ(22, 3)	1165.286796 (500)	-219	604	rP(22, 4)	1167.529955 (30)	162	654	pQ(3, 2)	1172.742620 (30)	72	704	pQ(11, 1)	1177.829606 (30)	-13
505	pP(10, 1)	1160.965836 (30)	-43	555	pQ(22, 3)	1165.293727 (500)	-210	605	pP(3, 2)	1167.655775 (30)	-2	655	pQ(2, 2)	1172.765923 (30)	-51	705	rP(10, 2)	1177.872865 (30)	-11
506	pQ(14, 4)	1160.981945 (30)	-5	556	pQ(21, 3)	1165.460652 (-)*	-112	606	rP(25, 5)	1167.711906 (200)	119	656	rP(16, 3)	1172.807836 (30)	4	706	pQ(10, 1)	1177.915478 (30)	42
507	pQ(13, 4)	1161.092087 (30)	-55	557	pQ(21, 3)	1165.466318 (-)*	-232	607	rP(28, 6)	1167.870020 (100)	18	657	rP(19, 4)	1173.074559 (30)	63	707	pQ(9, 1)	1177.993465 (30)	29
508	pQ(12, 4)	1161.194410 (30)	-13	558	rP(20, 3)	1165.482384 (30)	114	608	pP(6, 1)	1168.007685 (30)	-40	658	pP(3, 1)	1173.210428 (30)	19	708	pQ(8, 1)	1178.063608 (30)	-15
509	rP(13, 0)	1161.225838 (30)	76	559	pQ(20, 3)	1165.626394 (-)*	-95	609	rP(9, 0)	1168.343759 (30)	10	659	rP(22, 5)	1173.316068 (100)	143	709	pQ(7, 1)	1178.125986 (30)	-15
510	pQ(11, 4)	1161.288836 (30)	33	560	pQ(20, 3)	1165.631133 (-)*	-151	610	rP(12, 1)	1168.633501 (30)	-15	660	rP(25, 6)	1173.532161 (100)	20	710	pQ(6, 1)	1178.180589 (30)	15
511	pQ(10, 4)	1161.375330 (30)	42	561	rP(23, 4)	1165.668253 (30)	201	611	rP(15, 2)	1168.908554 (30)	17	661	rP(6, 0)	1173.607845 (30)	5	711	pQ(5, 1)	1178.228115 (1000)	771
512	rP(16, 1)	1161.418445 (30)	123	562	pQ(19, 3)	1165.784155 (-)*	-53	612	rP(18, 3)	1169.158949 (30)	67	662	rP(28, 7)	1173.722977 (-)*	-26	712	rP(13, 3)	1178.228115 (1000)	-477
513	pQ(9, 4)	1161.453792 (30)	-95	563	pQ(19, 3)	1165.787817 (-)*	-325	613	pP(2, 2)	1169.374753 (500)	41	663	rP(9, 1)	1173.969377 (30)	-11	713	pQ(4, 1)	1178.266296 (30)	-20
514	pQ(8, 4)	1161.524618 (30)	11	564	rP(26, 5)	1165.830630 (200)	99	614	rP(21, 4)	1169.384880 (500)	68	664	rP(12, 2)	1174.308669 (30)	-20	714	pQ(3, 1)	1178.297432 (30)	-58
515	pQ(7, 4)	1161.587382 (30)	-70	565	pP(4, 2)	1165.929230 (-)*	52	615	rP(24, 5)	1169.586491 (500)	22	665	rP(15, 3)	1174.621891 (30)	71	715	pQ(2, 1)	1178.320758 (1000)	-111
516	rP(19, 2)	1161.609776 (30)	95	566	pQ(18, 3)	1165.933919 (-)*	-16	616	pQ(28, 2)	1169.605870 (500)	-371	666	rP(18, 4)	1174.909170 (30)	100	716	pQ(1, 1)	1178.336605 (1000)	150
517	pQ(6, 4)	1161.642473 (30)	43	567	pQ(18, 3)	1165.936730 (-)*	-399	617	pP(5, 1)	1169.749441 (30)	-83	667	pP(2, 1)	1174.929401 (30)	0	717	rP(16, 4)	1178.557476 (30)	24
518	pQ(5, 4)	1161.689601 (30)	56	568	rP(29, 6)	1165.969721 (200)	4	618	rP(27, 6)	1169.763957 (200)	90	668	pQ(29, 1)	1174.940986 (200)	-313	718	rP(3, 0)	1178.806975 (30)	-2
519	pQ(4, 4)	1161.728754 (200)	-46	569	pQ(17, 3)	1166.077376 (2000)	1690	619	pQ(27, 2)	1169.826320 (200)	-234	669	pQ(28, 1)	1175.170114 (2000)	1203	719	rP(19, 5)	1178.859682 (40)	44
520	rP(22, 3)	1161.778494 (30)	136	570	pQ(17, 3)	1166.077376 (2000)	-872	620	pQ(26, 2)	1170.038639 (30)	-257	670	rP(21, 5)	1175.170114 (2000)	-491	720	pR(6, 3)	1178.978000 (200)	56
521	rP(25, 4)	1161.924821 (100)	238	571	pQ(16, 3)	1166.210580 (2000)	1104	621	rP(8, 0)	1170.105620 (30)	25	671	rP(5, 0)	1175.348145 (30)	-14	721	pR(6, 3)	1178.978002 (200)	-26
522	rP(28, 5)	1162.048454 (330)	-33	572	pQ(16, 3)	1166.210584 (2000)	-920	622	pQ(25, 2)	1170.243056 (30)	-221	672	pQ(27, 1)	1175.388582 (30)	0	722	rP(22, 6)	1179.135333 (40)	138
523	pP(3, 3)	1162.143440 (-)*	-6	573	pP(7, 1)	1166.258449 (30)	34	623	rP(11, 1)	1170.419417 (30)	8	673	rP(24, 6)	1175.406577 (100)	123	723	rP(6, 1)	1179.239168 (30)	13
524	pP(3, 3)	1162.143441 (-)*	-6	574	pQ(15, 3)	1166.336120 (2000)	801	624	pQ(24, 2)	1170.439571 (30)	-136	674	pQ(26, 1)	1175.600234 (30)	-86	724	rP(25, 7)	1179.383892 (500)	-119
525	rP(31, 6)	1162.150068 (-)*	-12	575	pQ(15, 3)	1166.336121 (2000)	-778	625	pQ(23, 2)	1170.628054 (30)	-140	675	rP(27, 7)	1175.616916 (-)*	432	725	pR(3, 2)	1179.524187 (-)*	-496
526	pP(6, 2)	1162.453151 (30)	-19	576	pQ(14, 3)	1166.453817 (2000)	589	626	rP(14, 2)	1170.715721 (30)	11	676	pR(4, 3)	1175.674897 (2000)	23	726	rP(9, 2)	1179.644075 (30)	17
527	pP(9, 1)	1162.737462 (30)	14	577	pQ(14, 3)	1166.453817 (2000)	-622	627	pQ(22, 2)	1170.808520 (30)	-229	677	pR(4, 3)	1175.674897 (2000)	-0	727	rQ(32, 0)	1179.702625 (1000)	-263
528	rP(12, 0)	1163.015831 (30)	54	578	pQ(13, 3)	1166.563649 (2000)	434	628	pQ(21, 2)	1170.981288 (-)*	-92	678	rP(8, 1)	1175.733383 (30)	-1	728	rQ(31, 0)	1179.958128 (100)	-58
529	rP(15, 1)	1163.232776 (30)	2	579	pQ(13, 3)	1166.563649 (2000)	-477	629	rP(17, 3)	1170.986895 (-)*	57	679	pQ(25, 1)	1175.804013 (1000)	-120	729	rP(12, 3)	1180.021326 (30)	41
530	rP(18, 2)	1163.444857 (30)	27	580	rP(10, 0)	1166.574845 (30)	39	630	pQ(20, 2)	1171.145951 (30)	-145	680	pQ(24, 1)	1175.999899 (30)	-129	730	rQ(30, 0)	1180.205651 (30)	-47
531	rP(21, 3)	1163.633854 (-)*	150	581	pQ(12, 3)	1166.665618 (2000)	324	631	rP(20, 4)	1171.233043 (30)	-18	681	rP(11, 2)	1176.094424 (30)	19	731	rP(15, 4)	1180.371183 (30)	16
532	rP(24, 4)	1163.799749 (100)	116	582	pQ(12, 3)	1166.665618 (2000)	-345	632	pQ(19, 2)	1171.302802 (30)	-104	682	pQ(23, 1)	1176.187967 (30)	-48	732	rQ(29, 0)	1180.445451 (30)	48
533	pQ(29, 3)	1163.844587 (500)	-116	583	pQ(11, 3)	1166.759700 (1000)	224	633	pQ(18, 2)	1171.451873 (500)	56	683	pQ(22, 1)	1176.368109 (30)	10	733	rP(2, 0)	1180.525340 (200)	-49
534	pQ(29, 3)	1163.864102 (500)	-550	584	pQ(11, 3)	1166.759703 (1000)	-251	634	pP(4, 1)	1171.483760 (30)	-8	684	rP(14, 3)	1176.428778 (30)	23	734	pR(7, 3)	1180.617120 (500)	-101
535	rP(27, 5)	1163.942791 (200)	42	585	rP(13, 1)	1166.840459 (-)*	43	635	pQ(17, 2)	1171.592784 (30)	-55	685	pQ(21, 1)	1176.540194 (30)	-96	735	pR(7, 3)	1180.617120 (500)	-242
536	rP(30, 6)	1164.063232 (200)	172	586	pQ(10, 3)	1166.845909 (1000)	139	636	rP(26, 6)	1171.651336 (100)	74	686	pP(1, 1)	1176.640638 (30)	-58	736	rQ(28, 0)	1180.677422 (30)	139
537	pQ(28, 3)	1164.074731 (500)	-361	587	pQ(10, 3)	1166.845909 (1000)	-193	637	pQ(16, 2)	1171.725952 (30)	-28	687	pQ(20, 1)	1176.704563 (30)	-32	737	rP(18, 5)	1180.694057 (40)	161
538	pQ(28, 3)	1164.092288 (500)	-255	588	pQ(9, 3)	1166.924289 (200)	102	638	rP(29, 7)	1171.822992 (300)	-116	688	rP(17, 4)	1176.736837 (30)	99	738	rQ(27, 0)	1180.901428 (30)	107
539	pP(5, 2)	1164.194962 (30)	2	589	pQ(9, 3)	1166.924289 (200)	-120	639	pQ(15, 2)	1171.851182 (30)	-64	689	pQ(19, 1)	1176.860899 (100)	-121	739	rP(5, 1)	1180.980735 (500)	-103
540	pQ(27, 3)	1164.297070 (200)	-267	590	pQ(8, 3)	1166.994799 (200)	62	640	rP(7, 0)	1171.860262 (100)	-44	690	pQ(18, 1)	1177.009517 (1000)	-58	740	rP(21, 6)	1180.989555 (500)	27
541	pQ(27, 3)	1164.312180 (200)	-344	591	pQ(8, 3)	1166.994799 (200)	-79	641	pQ(14, 2)	1171.968641 (30)	-5	691	rP(20, 5)	1177.018507 (1000)	-18	741	rQ(26, 0)	1181.117585 (30)	87
542	pP(8, 1)	1164.501646 (30)	5	592	pQ(7, 3)	1167.057506 (200)	80	642	pQ(13, 2)	1172.078181 (30)	-5	692	rP(4, 0)	1177.081182 (30)	-37	742	pR(4, 2)	1181.188733 (-)*	119
543	pQ(26, 3)	1164.511097 (1000)	-358	593	pQ(7, 3)	1167.057506 (200)	-5	643	pQ(12, 2)	1172.179808 (30)	-65	693	pQ(17, 1)	1177.150285 (30)	21	743	rP(24, 7)	1181.257843 (100)	-116
544	pQ(26, 3)	1164.524253 (1000)	-347	594	rP(16, 2)	1167.094340 (30)	37	644	rP(10, 1)	1172.198017 (30)	-31	694	rP(23, 6)	1177.274113 (500)	-42	744	rQ(25, 0)	1181.325852 (30)	53
545	pQ(25, 3)	1164.717218 (500)	-246	595	pQ(6, 3)	1167.112326 (100)	63	645	pQ(11, 2)	1172.273662 (30)	-51	695	pQ(16, 1)	1177.283051 (500)	-46	745	rP(8, 2)	1181.407844 (30)	-59
546	pQ(25, 3)	1164.728479 (500)	-296	596	pQ(6, 3)	1167.112326 (100)	15	646	pQ(10, 2)	1172.359674 (30)	-38	696	pR(5, 3)	1177.330435 (200)	-41	746	rQ(24, 0)	1181.526237 (30)	29
547	rP(11, 0)	1164.798855 (30)	52	597	pQ(5, 3)	1167.159267 (30)	12	647	pQ(9, 2)	1172.437852 (30)	-23	697	pR(5, 3)	1177.330435 (200)	-88	747	rQ(23, 0)	1181.718803 (30)	93
548	pQ(24, 3)	1164.915270 (200)	-113	598	pQ(5, 3)	1167.159267 (30)	-11	648	pQ(8, 2)	1172.508225 (200)	18	698	pQ(15, 1)	1177.408096 (30)	18	748	pR(1, 1)	1181.728519 (-)*	595
549	pQ(24, 3)	1164.924787 (200)	-267	599	pQ(4, 3)	1167.198439 (30)	34	649	rP(13, 2)	1172.515739 (200)	-37	699	rP(7, 1)	1177.489978 (30)	-11	749	rP(11, 3)	1181.806748 (30)	-40
550	rP(14, 1)	1165.040164 (30)	10	600	pQ(4, 3)	1167.198439 (30)	24	650	pQ(7, 2)	1172.570681 (30)	-32	700	rP(26, 7)	1177.503491 (300)	-12	750	rQ(22, 0)	1181.903343 (30)	51

TABLE A1—*Continued*

Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc	Line	Transition	Observed	Obs-Calc
751	rQ(21, 0)	1182.079965 (30)	26	801	rP(15, 5)	1186.155132 (100)	51	851	rP(6, 3)	1190.624731 (1000)	-89	901	rP(10, 5)	1195.115637 (2000)	26	951	rQ(6, 3)	1200.796502 (30)	18
752	rP(14, 4)	1182.177941 (200)	104	802	rQ(29, 1)	1186.187895 (500)	299	852	rR(3, 0)	1190.678949 (30)	12	902	rQ(5, 2)	1195.132430 (30)	-60	952	rQ(5, 3)	1200.843046 (30)	13
753	pR(8, 3)	1182.248630 (500)	377	803	rQ(28, 1)	1186.414290 (200)	360	853	rP(22, 8)	1190.866910 (-)*	323	903	rQ(4, 2)	1195.171347 (30)	41	953	rQ(4, 3)	1200.881826 (30)	4
754	pR(8, 3)	1182.248630 (500)	156	804	rP(18, 6)	1186.511839 (500)	35	854	pR(10, 2)	1191.001385 (-)*	184	904	rQ(3, 2)	1195.202291 (100)	-67	954	rP(10, 6)	1200.930746 (200)	-183
755	rQ(20, 0)	1182.248630 (30)	-10	805	rQ(27, 1)	1186.632811 (200)	417	855	rP(9, 4)	1191.103878 (500)	0	905	rP(13, 6)	1195.577002 (100)	-20	955	rR(6, 1)	1201.279969 (100)	67
756	rQ(19, 0)	1182.409364 (30)	-17	806	rP(5, 2)	1186.655004 (200)	49	856	rQ(32, 2)	1191.140897 (-)*	345	906	rR(6, 0)	1195.652547 (30)	-6	956	rP(13, 7)	1201.424726 (1000)	95
757	rP(17, 5)	1182.521197 (40)	-57	807	pR(4, 1)	1186.744322 (200)	186	857	rQ(31, 2)	1191.390285 (-)*	203	907	rP(16, 7)	1196.007691 (-)*	110	957	rP(16, 8)	1201.885584 (1000)	-403
758	rQ(18, 0)	1182.562139 (30)	-14	808	rP(21, 7)	1186.842966 (-)*	3009	858	rP(12, 5)	1191.552954 (200)	57	908	rR(3, 1)	1196.311281 (30)	-71	958	rR(3, 2)	1201.984709 (30)	32
759	rQ(17, 0)	1182.706927 (30)	-18	809	rQ(26, 1)	1186.842966 (-)*	-29	859	rQ(30, 2)	1191.632346 (-)*	594	909	rP(19, 8)	1196.407019 (-)*	-102	959	rR(10, 0)	1202.173742 (30)	12
760	rP(4, 1)	1182.714997 (2000)	8	810	rQ(25, 1)	1187.045856 (100)	116	860	pR(7, 1)	1191.688020 (200)	38	910	pR(10, 1)	1196.558031 (500)	-43	960	rP(19, 9)	1202.314658 (1000)	-27
761	rP(20, 6)	1182.837142 (2000)	37	811	rP(8, 3)	1187.119689 (100)	-1	861	rQ(29, 2)	1191.865757 (-)*	191	911	rP(9, 5)	1196.885966 (500)	-112	961	rQ(32, 4)	1202.604854 (1000)	-173
762	rQ(16, 0)	1182.843747 (2000)	1	812	rQ(24, 1)	1187.240779 (100)	144	862	rP(15, 6)	1191.971902 (100)	-103	912	rQ(31, 3)	1197.105396 (500)	586	962	rP(9, 6)	1202.701046 (1000)	-31
763	pR(5, 2)	1182.843747 (2000)	-742	813	rR(1, 0)	1187.324645 (100)	6	863	rQ(28, 2)	1192.091877 (200)	347	913	rR(7, 0)	1197.294813 (30)	31	963	rQ(31, 4)	1202.853763 (1000)	-80
764	rQ(15, 0)	1182.972523 (30)	-23	814	rQ(23, 1)	1187.427785 (100)	100	864	rQ(27, 2)	1192.310002 (200)	353	914	rQ(30, 3)	1197.346517 (500)	406	964	rR(7, 1)	1202.919882 (100)	-41
765	rQ(14, 0)	1183.093292 (30)	-46	815	rP(11, 4)	1187.554989 (100)	-121	865	rR(4, 0)	1192.344604 (30)	30	915	rP(12, 6)	1197.369034 (500)	180	965	rQ(30, 4)	1203.095276 (1000)	426
766	rP(23, 7)	1183.125223 (1000)	-75	816	rQ(22, 1)	1187.606951 (100)	54	866	rP(18, 7)	1192.360867 (-)*	-308	916	rQ(29, 3)	1197.579879 (200)	296	966	rP(12, 7)	1203.215872 (1000)	-237
767	rP(7, 2)	1183.164307 (30)	-58	817	pR(8, 2)	1187.763399 (500)	141	867	rP(5, 3)	1192.365811 (-)*	-392	917	rQ(28, 3)	1197.805528 (200)	300	967	rQ(29, 4)	1203.328390 (1000)	342
768	rQ(13, 0)	1183.206097 (30)	-17	818	rQ(21, 1)	1187.778389 (100)	113	868	rQ(26, 2)	1192.520097 (100)	169	918	rP(15, 7)	1197.820546 (500)	226	968	rQ(28, 4)	1203.553584 (500)	142
769	rQ(12, 0)	1183.310852 (30)	-12	819	rQ(20, 1)	1187.941878 (30)	50	869	rP(21, 8)	1192.722433 (-)*	2230	919	rR(4, 1)	1197.975594 (200)	27	969	rR(4, 2)	1203.648803 (30)	-39
770	rQ(11, 0)	1183.407582 (1000)	-2	820	rP(14, 5)	1187.961452 (100)	5	870	rQ(25, 2)	1192.722433 (-)*	61	920	rQ(27, 3)	1198.023421 (200)	370	970	rQ(27, 4)	1203.771327 (500)	294
771	pR(2, 1)	1183.407582 (1000)	-369	821	rQ(19, 1)	1188.097604 (30)	47	871	rP(8, 4)	1192.867157 (200)	-141	921	rQ(26, 3)	1198.233285 (1000)	230	971	rR(11, 0)	1203.784066 (200)	134
772	rQ(10, 0)	1183.496265 (30)	-1	822	rQ(18, 1)	1188.245478 (30)	8	872	rQ(24, 2)	1192.917322 (200)	335	922	rP(18, 8)	1198.240047 (-)*	-279	972	rQ(26, 4)	1203.981015 (500)	191
773	rQ(9, 0)	1183.576853 (2000)	-51	823	rP(17, 6)	1188.338786 (30)	-45	873	rR(1, 1)	1192.959037 (30)	-40	923	rQ(25, 3)	1198.435500 (100)	256	973	rP(18, 9)	1204.147444 (1000)	-65
774	rP(10, 3)	1183.585037 (2000)	-17	824	rQ(17, 1)	1188.385642 (2000)	72	874	rQ(23, 2)	1193.103902 (30)	126	924	rP(21, 9)	1198.629689 (1000)	1180	974	rQ(25, 4)	1204.182875 (100)	57
775	rQ(8, 0)	1183.649449 (30)	-44	825	rP(4, 2)	1188.385642 (2000)	-3345	875	rQ(22, 2)	1193.282803 (30)	58	925	rQ(24, 3)	1198.629689 (1000)	67	975	rQ(24, 4)	1204.377136 (100)	119
776	rQ(7, 0)	1183.713990 (30)	-38	826	pR(5, 1)	1188.400145 (1000)	-48	876	pR(8, 1)	1193.319751 (200)	141	926	rQ(23, 3)	1198.816348 (30)	155	976	rR(8, 1)	1204.551748 (100)	-31
777	rQ(6, 0)	1183.770470 (30)	-36	827	rQ(16, 1)	1188.517886 (30)	24	877	rP(11, 5)	1193.338112 (200)	243	927	rR(8, 0)	1198.929141 (30)	47	977	rQ(23, 4)	1204.563575 (100)	152
778	rQ(5, 0)	1183.818930 (30)	8	828	rQ(15, 1)	1188.642414 (30)	64	878	rQ(21, 2)	1193.454063 (200)	164	928	rQ(22, 3)	1198.995153 (30)	192	978	rQ(22, 4)	1204.742201 (100)	161
779	rQ(4, 0)	1183.859240 (30)	-33	829	rP(20, 7)	1188.687446 (2000)	266	879	rQ(20, 2)	1193.617366 (30)	125	929	rP(11, 6)	1199.153616 (500)	110	979	rQ(21, 4)	1204.912960 (100)	90
780	pR(9, 3)	1183.871187 (2000)	204	830	rQ(14, 1)	1188.759088 (30)	50	880	rQ(19, 2)	1193.772916 (-)*	140	930	rQ(21, 3)	1199.166041 (200)	113	980	rQ(20, 4)	1205.076090 (500)	174
781	pR(9, 3)	1183.871187 (2000)	-127	831	rQ(13, 1)	1188.867928 (1000)	-2	881	rP(14, 6)	1193.778050 (-)*	-6	931	rQ(20, 3)	1199.329268 (30)	170	981	rQ(19, 4)	1205.231157 (30)	-23
782	rQ(3, 0)	1183.891497 (30)	-61	832	rP(7, 3)	1188.875923 (2000)	-44	882	rQ(18, 2)	1193.920562 (30)	54	932	rQ(19, 3)	1199.484615 (30)	139	982	rR(5, 2)	1205.304977 (30)	-23
783	rQ(2, 0)	1183.915797 (30)	24	833	rQ(12, 1)	1188.969053 (30)	23	883	rR(5, 0)	1194.002399 (30)	-66	933	rP(14, 7)	1199.626531 (-)*	512	983	rQ(18, 4)	1205.378753 (1000)	89
784	rQ(1, 0)	1183.931867 (30)	-50	834	rR(2, 0)	1189.005701 (30)	93	884	rQ(17, 2)	1194.060494 (30)	52	934	rR(5, 1)	1199.632126 (-)*	360	984	rR(12, 0)	1205.386062 (1000)	89
785	rP(13, 4)	1183.977493 (30)	78	835	rQ(11, 1)	1189.062380 (30)	40	885	rP(17, 7)	1194.188040 (-)*	190	935	rQ(18, 3)	1199.632126 (30)	63	985	rQ(17, 4)	1205.518410 (30)	40
786	rP(16, 5)	1184.341616 (100)	-49	836	rQ(10, 1)	1189.147863 (30)	-1	886	rQ(16, 2)	1194.192590 (-)*	10	936	rQ(17, 3)	1199.771943 (200)	80	986	rQ(16, 4)	1205.650298 (30)	-4
787	rP(3, 1)	1184.441427 (-)*	-135	837	rQ(9, 1)	1189.225595 (30)	-9	887	rQ(15, 2)	1194.316970 (30)	44	937	rQ(16, 3)	1199.903995 (30)	115	987	rQ(15, 4)	1205.774462 (30)	1
788	pR(6, 2)	1184.492384 (-)*	128	838	rQ(8, 1)	1189.295612 (30)	49	888	rQ(14, 2)	1194.433572 (30)	88	938	rQ(15, 3)	1200.028179 (30)	64	988	rQ(14, 4)	1205.890892 (30)	43
789	rP(19, 6)	1184.677959 (30)	79	839	rP(10, 4)	1189.333055 (100)	-78	889	rQ(13, 2)	1194.542251 (30)	-6	939	rP(17, 8)	1200.067078 (-)*	448	989	rP(17, 9)	1205.973236 (1000)	-191
790	rP(6, 2)	1184.913522 (100)	124	840	rQ(7, 1)	1189.357646 (30)	-97	890	rP(20, 8)	1194.567186 (-)*	122	940	rQ(14, 3)	1200.144569 (30)	-3	990	rQ(13, 4)	1205.999436 (30)	-33
791	rP(22, 7)	1184.985881 (100)	-99	841	pR(9, 2)	1189.386122 (1000)	-267	891	rP(7, 4)	1194.624093 (-)*	748	941	rQ(13, 3)	1200.253272 (30)	19	991	rQ(12, 4)	1206.100313 (30)	-9
792	pR(3, 1)	1185.079991 (100)	-48	842	rQ(6, 1)	1189.412140 (30)	-7	892	rR(2, 1)	1194.639268 (-)*	95	942	rR(2, 2)	1200.312552 (30)	-3	992	rR(9, 1)	1206.175346 (100)	-74
793	rP(9, 3)	1185.356001 (30)	-36	843	rQ(5, 1)	1189.458720 (30)	-55	893	rQ(12, 2)	1194.643163 (-)*	-84	943	rQ(12, 3)	1200.354247 (30)	86	993	rQ(11, 4)	1206.193435 (30)	25
794	pR(10, 3)	1185.485590 (500)	237	844	rQ(4, 1)	1189.497533 (30)	-97	894	rQ(11, 2)	1194.736466 (30)	7	944	rQ(11, 3)	1200.447316 (30)	18	994	rQ(10, 4)	1206.278805 (30)	71
795	pR(10, 3)	1185.485592 (500)	240	845	rQ(3, 1)	1189.528652 (30)	-60	895	rQ(10, 2)	1194.821953 (30)	60	945	rP(20, 9)	1200.474856 (-)*	-146	995	rQ(9, 4)	1206.356247 (30)	-50
796	rR(0, 0)	1185.635902 (200)	180	846	rQ(2, 1)	1189.552162 (100)	139	896	rQ(9, 2)	1194.899608 (30)	55	946	rQ(10, 3)	1200.532689 (30)	23	996	rQ(8, 4)	1206.426154 (30)	55
797	rQ(31, 1)	1185.711872 (500)	579	847	rP(13, 5)	1189.760586 (100)	-158	897	pR(9, 1)	1194.943141 (-)*	149	947	rR(9, 0)	1200.555524 (30)	94	997	rQ(7, 4)	1206.488221 (30)	79
798	rP(12, 4)	1185.769769 (30)	-86	848	pR(6, 1)	1190.048056 (100)	-103	898	rQ(8, 2)	1194.969475 (30)	34	948	rQ(9, 3)	1200.610289 (30)	22	998	rQ(6, 4)	1206.542490 (100)	63
799	rQ(30, 1)	1185.953612 (200)	226	849	rP(16, 6)	1190.158975 (100)	61	899	rQ(7, 2)	1195.031565 (30)	6	949	rQ(8, 3)	1200.680144 (30)	42	999	rQ(5, 4)	1206.588918 (100)	-38
800	pR(7, 2)	1186.132013 (500)	150	850	rP(19, 7)	1190.527430 (1000)	-172	900	rQ(6, 2)	1195.085945 (30)	37	950	rQ(7, 3)	1200.742198 (30)	24	1000	rR(6, 2)	1206.953021 (30)	-81

TABLE A1—*Continued*

Line	Transition	Observed	Obs-Calc
1001	rR(13, 0)	1206.979815 (200)	25
1002	rR(3, 3)	1207.694629 (30)	22
1003	rR(10, 1)	1207.790994 (2000)	199
1004	rP(16, 9)	1207.790994 (2000)	-1395
1005	rR(14, 0)	1208.565270 (200)	-47
1006	rR(7, 2)	1208.593036 (100)	-61
1007	rQ(31, 5)	1208.636264 (-)*	597
1008	rQ(30, 5)	1208.876984 (-)*	531
1009	rQ(29, 5)	1209.109925 (-)*	473
1010	rQ(28, 5)	1209.335046 (1000)	382
1011	rR(4, 3)	1209.358735 (30)	83
1012	rR(11, 1)	1209.397959 (200)	106
1013	rQ(27, 5)	1209.552032 (200)	-58
1014	rP(15, 9)	1209.604643 (-)*	294
1015	rQ(26, 5)	1209.761833 (200)	101
1016	rQ(25, 5)	1209.963740 (230)	148
1017	rR(15, 0)	1210.142600 (200)	111
1018	rQ(24, 5)	1210.157903 (200)	233
1019	rR(8, 2)	1210.225029 (100)	92
1020	rQ(23, 5)	1210.344178 (200)	210
1021	rQ(22, 5)	1210.522696 (100)	209
1022	rQ(21, 5)	1210.693333 (100)	103
1023	rQ(20, 5)	1210.856291 (100)	93
1024	rR(12, 1)	1210.996684 (500)	140
1025	rQ(19, 5)	1211.014602 (2000)	3210
1026	rR(5, 3)	1211.014602 (2000)	-95
1027	rQ(18, 5)	1211.158930 (100)	115
1028	rQ(17, 5)	1211.298469 (30)	2
1029	rQ(16, 5)	1211.430396 (30)	45
1030	rQ(15, 5)	1211.554507 (30)	39
1031	rQ(14, 5)	1211.670880 (30)	61
1032	rQ(13, 5)	1211.779447 (30)	41
1033	rR(9, 2)	1211.848616 (30)	46
1034	rQ(12, 5)	1211.880143 (30)	-88
1035	rQ(11, 5)	1211.973266 (30)	-29
1036	rQ(10, 5)	1212.058564 (30)	-34
1037	rQ(9, 5)	1212.136153 (30)	10
1038	rQ(8, 5)	1212.206017 (30)	87
1039	rQ(7, 5)	1212.267989 (30)	29
1040	rQ(6, 5)	1212.322224 (100)	-10
1041	rR(13, 1)	1212.586690 (200)	-124
1042	rR(6, 3)	1212.662714 (30)	22
1043	rR(10, 2)	1213.463903 (130)	-44
1044	rR(14, 1)	1214.168577 (200)	-36
1045	rQ(32, 6)	1214.200215 (-)*	-71
1046	rR(7, 3)	1214.302601 (30)	15
1047	rQ(31, 6)	1214.449244 (-)*	542
1048	rQ(30, 6)	1214.689871 (-)*	523
1049	rQ(29, 6)	1214.922502 (-)*	278
1050	rR(11, 2)	1215.071051 (100)	34
1051	rR(4, 4)	1215.103566 (30)	16
1052	rQ(28, 6)	1215.147581 (100)	254
1053	rQ(27, 6)	1215.364846 (200)	187
1054	rQ(26, 6)	1215.574330 (200)	111
1055	rR(15, 1)	1215.742035 (-)*	146
1056	rQ(25, 6)	1215.776134 (100)	127
1057	rR(8, 3)	1215.934351 (30)	19
1058	rQ(24, 6)	1215.970166 (100)	142
1059	rQ(23, 6)	1216.156356 (30)	85
1060	rQ(22, 6)	1216.334888 (30)	141
1061	rQ(21, 6)	1216.505615 (30)	162
1062	rQ(20, 6)	1216.668702 (1000)	311
1063	rR(12, 2)	1216.668702 (1000)	-1026
1064	rR(5, 4)	1216.759470 (30)	60
1065	rQ(19, 6)	1216.823501 (30)	-60
1066	rQ(18, 6)	1216.970977 (30)	13
1067	rQ(17, 6)	1217.110640 (30)	39
1068	rQ(16, 6)	1217.242403 (30)	-70
1069	rR(16, 1)	1217.306666 (1000)	77
1070	rQ(15, 6)	1217.366623 (30)	42
1071	rQ(14, 6)	1217.482907 (30)	-20
1072	rR(9, 3)	1217.557925 (30)	47
1073	rQ(13, 6)	1217.591516 (30)	6
1074	rQ(12, 6)	1217.692388 (30)	55
1075	rQ(11, 6)	1217.785462 (30)	66
1076	rQ(10, 6)	1217.870815 (30)	115
1077	rQ(9, 6)	1217.948280 (30)	33
1078	rQ(8, 6)	1218.018177 (30)	141
1079	rQ(7, 6)	1218.080144 (100)	76
1080	rR(13, 2)	1218.259954 (100)	-77
1081	rR(6, 4)	1218.407200 (30)	-24
1082	rR(10, 3)	1219.173162 (30)	-14
1083	rR(14, 2)	1219.841729 (500)	-144
1084	rR(7, 4)	1220.046880 (30)	-63
1085	rR(11, 3)	1220.780158 (30)	-16
1086	rQ(28, 7)	1220.989677 (-)*	-109
1087	rQ(27, 7)	1221.207758 (-)*	659
1088	rR(15, 2)	1221.415789 (2000)	586
1089	rQ(26, 7)	1221.415789 (2000)	-859
1090	rQ(25, 7)	1221.618543 (500)	110
1091	rR(8, 4)	1221.678598 (30)	80
1092	rQ(24, 7)	1221.812622 (500)	169
1093	rQ(23, 7)	1221.998609 (500)	-99
1094	rQ(22, 7)	1222.177202 (100)	6
1095	rQ(21, 7)	1222.347820 (100)	-99
1096	rR(12, 3)	1222.378927 (30)	105
1097	rQ(20, 7)	1222.510908 (100)	32
1098	rR(5, 5)	1222.537728 (30)	91
1099	rQ(19, 7)	1222.666023 (100)	-45
1100	rQ(18, 7)	1222.813454 (100)	-40
1101	rQ(17, 7)	1222.953164 (100)	9
1102	rR(16, 2)	1222.979911 (500)	-58
1103	rQ(16, 7)	1223.084989 (100)	-64
1104	rQ(15, 7)	1223.209272 (100)	85
1105	rR(9, 4)	1223.301925 (100)	27
1106	rQ(14, 7)	1223.325634 (100)	77
1107	rQ(13, 7)	1223.434055 (100)	-111
1108	rQ(12, 7)	1223.534914 (100)	-99
1109	rQ(11, 7)	1223.628064 (100)	-35
1110	rQ(10, 7)	1223.713228 (100)	-198
1111	rQ(9, 7)	1223.791119 (100)	127
1112	rQ(8, 7)	1223.861400 (500)	600
1113	rR(13, 3)	1223.969057 (100)	-13
1114	rR(6, 5)	1224.185270 (100)	71
1115	rR(10, 4)	1224.917112 (30)	78
1116	rR(14, 3)	1225.550776 (100)	-91
1117	rR(7, 5)	1225.824788 (100)	120
1118	rR(11, 4)	1226.523864 (30)	-13
1119	rQ(27, 8)	1227.077509 (-)*	-180
1120	rR(15, 3)	1227.124343 (100)	180
1121	rQ(26, 8)	1227.287387 (-)*	80
1122	rR(8, 5)	1227.455984 (500)	-10
1123	rQ(25, 8)	1227.489156 (500)	-7
1124	rQ(24, 8)	1227.683050 (500)	-205
1125	rQ(23, 8)	1227.869497 (500)	-86
1126	rQ(22, 8)	1228.048285 (200)	140
1127	rR(12, 4)	1228.122619 (100)	243
1128	rQ(21, 8)	1228.218967 (200)	26
1129	rQ(20, 8)	1228.381733 (200)	-237
1130	rQ(19, 8)	1228.537276 (100)	45
1131	rQ(18, 8)	1228.684809 (-)*	83
1132	rR(16, 3)	1228.688857 (-)*	-48
1133	rQ(17, 8)	1228.824265 (200)	-188
1134	rQ(16, 8)	1228.956396 (200)	-18
1135	rR(9, 5)	1229.079551 (1000)	422
1136	rQ(15, 8)	1229.079551 (1000)	-1057
1137	rQ(14, 8)	1229.197011 (200)	-25
1138	rQ(13, 8)	1229.305637 (200)	-62
1139	rQ(12, 8)	1229.406434 (200)	-162
1140	rQ(11, 8)	1229.500009 (200)	280
1141	rQ(10, 8)	1229.585148 (200)	49
1142	rQ(9, 8)	1229.662535 (-)*	-170
1143	rR(13, 4)	1229.712358 (200)	-123
1144	rR(6, 6)	1229.995119 (30)	63
1145	rR(10, 5)	1230.694140 (100)	116
1146	rR(14, 4)	1231.294234 (200)	91
1147	rR(7, 6)	1231.634316 (30)	115
1148	rR(11, 5)	1232.300556 (100)	-72
1149	rQ(29, 9)	1232.532218 (-)*	428
1150	rQ(28, 9)	1232.757806 (-)*	718
1151	rR(15, 4)	1232.867238 (200)	-73
1152	rQ(27, 9)	1232.975213 (-)*	586
1153	rQ(26, 9)	1233.185190 (-)*	788
1154	rR(8, 6)	1233.265222 (30)	17
1155	rQ(25, 9)	1233.386650 (500)	237
1156	rQ(24, 9)	1233.580591 (200)	-64
1157	rQ(23, 9)	1233.767305 (200)	177
1158	rR(12, 5)	1233.898840 (100)	-53
1159	rQ(22, 9)	1233.945879 (200)	48
1160	rQ(21, 9)	1234.116662 (200)	-99
1161	rQ(20, 9)	1234.279959 (200)	41
1162	rR(16, 4)	1234.435177 (-)*	3242
1163	rQ(19, 9)	1234.435177 (-)*	-126
1164	rQ(18, 9)	1234.582591 (200)	-323
1165	rQ(17, 9)	1234.722689 (200)	-62
1166	rQ(16, 9)	1234.854689 (-)*	-126
1167	rR(9, 6)	1234.888019 (30)	1
1168	rQ(15, 9)	1234.979083 (100)	-23
1169	rQ(14, 9)	1235.095488 (100)	-137
1170	rQ(13, 9)	1235.204155 (100)	-216
1171	rQ(12, 9)	1235.305390 (100)	44
1172	rQ(11, 9)	1235.398730 (200)	180
1173	rQ(10, 9)	1235.483979 (-)*	-5
1174	rR(13, 5)	1235.488543 (-)*	-226
1175	rR(10, 6)	1236.502619 (30)	28
1176	rR(14, 5)	1237.070346 (200)	140
1177	rR(7, 7)	1237.474044 (30)	114
1178	rR(11, 6)	1238.108897 (30)	22
1179	rR(15, 5)	1238.643399 (200)	245
1180	rR(8, 7)	1239.104665 (30)	129
1181	rR(12, 6)	1239.706799 (30)	-22
1182	rR(16, 5)	1240.207548 (-)*	-16
1183	rR(9, 7)	1240.726913 (30)	-36
1184	rQ(16,10)	1240.778833 (-)*	381
1185	rQ(15,10)	1240.902834 (-)*	-45
1186	rQ(14,10)	1241.019727 (-)*	204
1187	rQ(13,10)	1241.128477 (-)*	92
1188	rQ(12,10)	1241.229624 (-)*	158
1189	rR(13, 6)	1241.296280 (100)	-100
1190	rR(10, 7)	1242.341212 (100)	91
1191	rR(14, 6)	1242.877466 (100)	-37
1192	rR(11, 7)	1243.946967 (100)	-37
1193	rR(15, 6)	1244.450221 (100)	81
1194	rR(8, 8)	1244.972367 (100)	54
1195	rR(12, 7)	1245.544510 (100)	-38
1196	rR(16, 6)	1246.014047 (100)	-195
1197	rR(9, 8)	1246.594197 (100)	-54
1198	rR(13, 7)	1247.133383 (200)	-321
1199	rR(10, 8)	1248.207676 (200)	-268
1200	rR(14, 7)	1248.714758 (200)	334
1201	rR(11, 8)	1249.813298 (200)	-45
1202	rR(15, 7)	1250.286709 (200)	51
1203	rR(12, 8)	1251.410483 (2000)	82
1204	rR(16, 7)	1251.850469 (1000)	111
1205	rQ(19,12)	1252.273234 (-)*	752
1206	rQ(18,12)	1252.421753 (1000)	974
1207	rR(9, 9)	1252.488350 (30)	160
1208	rR(13, 8)	1252.999071 (500)	3
1209	rR(17, 7)	1253.405537 (500)	62
1210	rR(10, 9)	1254.101420 (30)	95
1211	rR(14, 8)	1254.579430 (500)	135
1212	rR(18, 7)	1254.951995 (500)	35
1213	rR(11, 9)	1255.706232 (100)	72
1214	rR(15, 8)	1256.150909 (200)	-125
1215	rR(12, 9)	1257.302710 (100)	63
1216	rR(16, 8)	1257.714362 (200)	125
1217	rR(13, 9)	1258.890853 (200)	115
1218	rR(10,10)	1260.019570 (200)	98
1219	rR(14, 9)	1260.470378 (200)	-4
1220	rR(11,10)	1261.623797 (200)	136
1221	rR(15, 9)	1262.041528 (200)	-4
1222	rR(12,10)	1263.219491 (200)	-1
1223	rR(16, 9)	1263.604180 (200)	40
1224	rR(13,10)	1264.806986 (500)	69
1225	rR(17, 9)	1265.158094 (500)	-61
1226	rR(18, 9)	1266.703635 (500)	104
1227	rR(11,11)	1267.564257 (500)	267
1228	rR(12,11)	1269.159249 (500)	170
1229	rR(13,11)	1270.745886 (500)	137
1230	rR(12,12)	1275.119833 (500)	343
1231	rR(13,12)	1276.705713 (500)	400
1232	rR(14,12)	1278.282988 (500)	340

Note:
Numbers in parentheses represent estimated experimental uncertainties in units of the last digit quoted. Asterisks denote experimental data which have not been included in the fit. The Obs-Calc values are given in the same units as experimental uncertainties.

TABLE A2

Comparison of Observed and Calculated Transition Frequencies of Purely Rotational Transitions in the $v_6 = 1$ State of $^{12}CH_3F$ (in MHz)

J	kl	Exp	Calc	Exp-Calc	J	kl	Exp	Calc	Exp-Calc
0	0	50837.75 (20)A	50837.57	18	6	1	355850.44 (20)	355850.16	28
					6	2	355786.31 (20)	355786.34	-3
1	0	101673.77 (20)B	101673.68	9	6	3	355769.66 (20)	355769.51	15
1	1	101659.03 (20)B	101658.68	35	6	4	355740.07 (20)	355739.94	14
1	1	101693.87 (20)B	101693.71	17	6	5	355697.73 (20)	355697.64	9
1	-1	101667.40 (20)B	101667.48	-8	6	6	355642.77 (20)	355642.68	9
					6	-1	355759.46 (20)	355759.48	-2
2	0	152506.86 (10)C	152506.87	-0	6	-2	355724.69 (20)	355724.72	-3
2	1	152484.32 (10)C	152484.45	-12	6	-3	355676.81 (20)	355676.95	-14
2	1	152536.99 (10)C	152536.85	14	6	-4	355615.94 (20)	355616.14	-20
2	2	152508.97 (10)C	152508.92	5	6	-5	355542.13 (20)	355542.24	-11
2	-1	152497.55 (10)C	152497.56	-2	6	-6	355455.21 (20)	355455.22	-1
2	-2	152482.66 (10)C	152482.71	-5					
					7	0	406578.13 (20)C	406577.97	16
3	0	203335.71 (10)C	203335.68	3	7	1	406520.22 (20)	406520.33	-11
3	1	203305.84 (10)	203305.92	-9	7	1	406656.53 (20)	406656.26	27
3	1	203375.75 (20)	203375.55	20	7	2	406584.04 (20)C	406583.90	14
3	2	203338.54 (20)	203338.45	10	7	3	406564.89 (20)	406564.69	20
3	3	203328.86 (20)	203328.81	5	7	4	406531.00 (20)	406530.91	9
3	-1	203323.28 (20)	203323.27	1	7	5	406482.79 (20)	406482.60	19
3	-2	203303.46 (10)C	203303.45	0	7	6	406419.96 (20)	406419.81	16
3	-3	203276.14 (10)C	203276.21	-7	7	7	406342.61 (20)	406342.59	2
					7	-1	406552.93 (20)C	406553.05	-12
4	0	-	254158.66		7	-2	406513.71 (200)	406513.28	43
4	1	254123.50 (300)	254121.68	182	7	-3	406458.49 (20)	406458.64	-15
4	1	254209.11 (300)	254208.33	78	7	-4	406388.87 (20)	406389.09	-22
4	2	254161.98 (20)	254162.16	-18	7	-5	406304.39 (20)	406304.58	-19
4	3	254150.24 (20)	254150.12	12	7	-6	406204.92 (20)	406205.07	-15
4	4	254129.07 (20)	254128.97	10	7	-7	406090.13 (100)	406090.52	-39
4	-1	-	254143.13						
4	-2	254118.44 (20)	254118.34	10	8	0	-	457363.01	
4	-3	254084.26 (20)	254084.27	-1	8	1	-	457298.90	
4	-4	254040.84 (20)	254040.88	-4	8	1	457450.72 (20)	457450.50	22
					8	2	-	457369.84	
5	0	-	304974.34		8	3	457348.44 (20)	457348.25	19
5	1	304932.55 (300)	304930.28	227	8	4	-	457310.28	
5	1	305033.92 (20)	305033.69	23	8	5	457256.20 (20)	457255.96	24
5	2	304978.77 (20)	304978.61	16	8	6	457185.46 (20)	457185.34	12
5	3	304964.31 (20)	304964.17	14	8	7	457098.53 (100)	457098.50	3
5	4	304938.94 (20)	304938.80	14	8	8	-	456995.50	
5	5	304902.72 (20)	304902.54	18	8	-1	457334.96 (20)	457334.93	3
5	-1	304955.68 (20)	304955.69	-1	8	-2	-	457290.14	
5	-2	-	304925.92		8	-3	457228.39 (20)	457228.61	-22
5	-3	304884.88 (20)C	304885.01	-12	8	-4	457150.00 (20)	457150.29	-29
5	-4	304832.82 (20)	304832.91	-9	8	-5	457054.79 (20)	457055.15	-36
5	-5	304769.58 (20)	304769.61	-3	8	-6	456942.76 (200)	456943.13	-37
					8	-7	456813.86 (200)	456814.18	-32
6	0	355781.36 (20)	355781.26	10	8	-8	456668.01 (200)	456668.27	-26
6	1	355730.07 (20)	355730.31	-24					
9	0	-	508134.91		10	-1	558858.95 (20)	558857.80	115
9	1	508064.43 (20)	508064.61	-18	10	-2	558804.83 (-)*	558802.90	193
9	1	508231.62 (20)	508231.40	22	10	-3	558728.46 (20)	558727.52	94
9	2	508142.54 (20)	508142.70	-16	10	-4	558632.29 (20)	558631.61	68

Our measurement unless stated otherwise: A(18), B(19), C(17). The J and kl values refer to quantum numbers of the lower state of the rotational transition. Numbers in parentheses represent estimated experimental uncertainties in units of the last digit quoted. Asterisks denote experimental data which have not included in the fit. The Exp-Calc values are given in the same units as experimental uncertainties.

TABLE A2—*Continued*

J	kl	Exp	Calc	Exp-Calc	J	kl	Exp	Calc	Exp-Calc
9	3	508118.91 (20)	508118.74	17	10	-5	558515.67 (20)	558515.12	55
9	4	-	508076.59		10	-6	558377.83 (20)	558377.98	-15
9	5	508016.48 (20)	508016.27	21	10	-7	558219.11 (20)	558220.15	-104
9	6	507938.04 (20)	507937.84	20	10	-8	558040.15 (20)	558041.58	-143
9	7	507841.48 (20)	507841.38	11	10	-9	557840.54 (200)	557842.20	-166
9	8	507726.96 (20)	507726.96	1	10	-10	-	557621.97	
9	9	507595.61 (200)	507594.66	95					
9	-1	508103.56 (20)	508103.67	-11	11	0	609633.73 (20)	609633.49	24
9	-2	508053.86 (20)	508053.83	3	11	1	609551.69 (20)	609551.69	0
9	-3	507985.07 (20)	507985.39	-32	11	1	609746.69 (20)	609747.26	-57
9	-4	507897.89 (20)	507898.29	-40	11	2	609643.10 (20)	609643.36	-27
9	-5	507792.04 (20)	507792.49	-45	11	3	609614.96 (20)	609614.71	25
9	-6	507667.35 (20)	507667.92	-57	11	4	609564.41 (20)	609564.24	17
9	-7	507523.75 (20)	507524.55	-80	11	5	609492.29 (20)	609491.95	34
9	-8	507361.41 (200)	507362.32	-91	11	6	609398.33 (20)	609397.93	40
9	-9	507180.07 (20)	507181.19	-112	11	7	609282.60 (20)	609282.25	35
					11	8	609145.36 (20)	609145.00	35
10	0	558896.86 (-)*	558892.23	463	11	9	608986.77 (20)	608986.29	47
10	1	-	558816.02		11	10	608806.42 (20)	608806.22	20
10	1	558998.67 (20)	558997.48	119	11	-1	609595.70 (20)	609595.87	-17
10	2	-	558901.02		11	-2	609536.20 (100)	609535.88	33
10	3	558876.10 (20)	558874.71	139	11	-3	609453.08 (20)	609453.53	-45
10	4	558828.46 (20)	558828.39	7	11	-4	609348.18 (20)	609348.79	-60
10	5	558763.83 (20)	558762.08	175	11	-5	609220.81 (20)	609221.57	-76
10	6	558677.20 (20)	558675.85	135	11	-6	609070.75 (20)	609071.84	-108
10	7	558571.13 (20)	558569.77	136	11	-7	608898.01 (20)	608899.51	-151
10	8	558445.07 (20)	558443.94	113	11	-8	608702.39 (20)	608704.55	-215
10	9	558300.30 (200)	558298.43	187	11	-9	608483.87 (200)	608486.88	-301
10	10	558133.73 (200)	558133.35	38	11	-10	608235.63 (-)*	608246.46	-1083

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