

## The Second Torsional State of Acetaldehyde

S. P. BELOV,\* M. YU. TRETYAKOV,\* I. KLEINER,† AND J. T. HOUGEN‡

\*Microwave Spectroscopy Division, Applied Physics Institute, 46 Ulyanova Street, Nizhny Novgorod, Russia 603024; †Laboratoire de Physique Moléculaire et Applications, Université Pierre et Marie Curie et C.N.R.S., Tour 13, 4, Place Jussieu, F-75252 Paris Cedex 05, France; and ‡Molecular Physics Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899

We have fit to within experimental accuracy a data set for acetaldehyde obtained by combining 1014  $v_t = 0$ , 840  $v_t = 1$ , and 430  $v_t = 2$  microwave lines with 420  $v_t = 1 \leftarrow 0$  and 404  $v_t = 2 \leftarrow 1$  far-infrared lines. The principal additions to the previously treated  $v_t = 0$  and  $v_t = 1$  microwave data set consist of about 250 new measurements from Barclay, Anderson, and Ziurys and 900 new measurements from Nizhny Novgorod; the  $v_t = 2$  measurements include about 400 lines from Nizhny Novgorod and a few lines from various other sources. The previously treated  $v_t = 1 \leftarrow 0$  far-infrared data set was extended by adding about 200 high- $J$  lines from the  $1 \leftarrow 0$  fundamental band and 400 lines from the  $2 \leftarrow 1$  hot band, all taken from a previously reported Fourier transform spectrum. The final fit, which uses a slightly extended model from the literature, requires 48 parameters to achieve an overall unitless weighted standard deviation of 1.06. The present fit includes essentially all available infrared and microwave transitions involving torsional levels below the top of the internal rotation barrier. © 1993 Academic Press, Inc.

### 1. INTRODUCTION

This is the fifth in a series of papers (1–4) on the infrared and microwave spectrum of acetaldehyde ( $\text{CH}_3\text{CHO}$ ). Reference (3) presents a global fit of 907 microwave and far-infrared transitions involving the ground and first torsional state. Reference (4) presents 257 new  $v_t = 0$  and 1 measurements (and one line reassigned to  $v_t = 2$ ) in the region from 240 to 350 GHz.

In this paper we present a larger global analysis which treats: (i) the 1165 microwave and millimeter transitions mentioned in the previous paragraph, (ii) 1315 new sub-millimeter transitions in the torsional states  $v_t = 0, 1$ , and 2, measured with the RAD-3 spectrometer in Nizhny Novgorod, (iii) 206 high- $J$  infrared transitions from the  $v_t = 1 \leftarrow 0$  torsional fundamental band reported in (1) but not included in the fit at that time, (iv) 404 new far-infrared transitions in the  $v_t = 2 \leftarrow 1$  hot band, assigned in the present work after a reexamination of the original Ottawa BOMEM spectrum (1), and (v) 18 miscellaneous  $v_t = 0, 1$ , and 2 lines measured at NIST (5). The total data set thus contains 3108 transitions (though some of these are unresolved  $K$ -type doublets counted twice).

Even though the  $v_t = 0$  and  $v_t = 1$  data sets were significantly enlarged in the present work, our actual goal was a study of the  $v_t = 2$  torsional level. This is the last level lying below the top of the torsional barrier, and as such, it corresponds neither to the high-barrier nor to the low-barrier limit. As shown below, we now have a rather good experimental and theoretical understanding of  $v_t = 2$  rotational levels for  $J \leq 26$ .

## 2. EXPERIMENTAL DETAILS

The new submillimeter wave measurements in the range from 164.8 to 417.4 GHz were recorded at room temperature with the RAD-3 spectrometer in Nizhny Novgorod (6), which uses a backward wave oscillator source, photoacoustic detection, and a Fabry-Perot cavity for frequency tuning to produce a broadband scan. The sample pressure of approximately 13 Pa (0.1 Torr) gave typical linewidths of 8 MHz, which when combined with some uncertainties in the  $\text{SO}_2$  frequencies used for calibration, led to measurement uncertainties of less than 1 MHz for unblended lines. A typical trace is illustrated in Fig. 1. About 5000 lines were recorded with RAD-3. Lines used in the fit were given a weight corresponding to a measurement uncertainty of  $\pm 1$  MHz.

The far-infrared measurements were all taken from the BOMEM Fourier transform spectrum first reported in Ref. (1). Again only unblended lines were retained for the fit. The high- $J$   $v_t = 1 \leftarrow 0$  lines ( $11 \leq J \leq 26$ ) are reported in Ref. (1), but were not included in the  $J \leq 10$  fit carried out at that time. The  $v_t = 2 \leftarrow 1$  hot band lines taken from the same spectrum were somewhat weaker, but these lines could gradually be assigned with certainty after various eigenvalue labeling problems in the computer program were solved, and the number of parameters adjusted in the fit was increased. Lines from the  $v_t = 1 \leftarrow 0$  fundamental band were given a weight corresponding to a measurement uncertainty of  $0.00035 \text{ cm}^{-1}$  (as in Ref. (3)); lines from the  $v_t = 2 \leftarrow 1$  hot band were given a weight corresponding to a measurement uncertainty of  $0.00050 \text{ cm}^{-1}$  to allow for the fact that they are weaker than lines in the fundamental band.

## 3. THEORETICAL MODEL

The theoretical model used earlier (1-3), which is based on the work of Refs. (7, 8), was also used in the present study after three changes were incorporated.

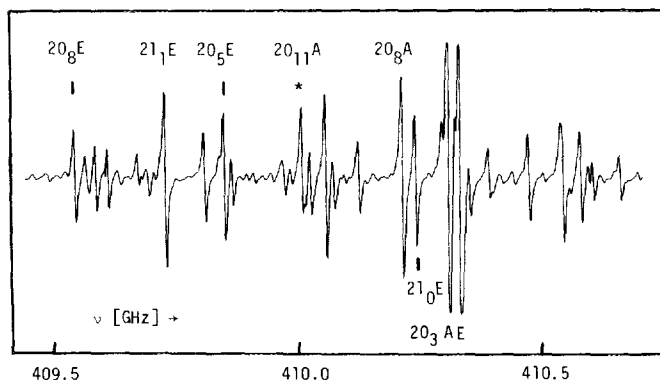


FIG. 1. A portion of the room-temperature submillimeter-wave spectrum of acetaldehyde between 409.5 and 410.5 GHz, recorded with the RAD-3 spectrometer in Nizhny Novgorod. The noise level is much smaller than the pen width. Five  $a$ -type lines originating in the  $v_t = 2$  state are labeled above the spectrum with lower-state quantum numbers  $J_K$  and symmetry species  $A$  or  $E$ . (For example, the first line is the  $21_8-20_8 E$  transition occurring at 409 545.3 MHz in Table II.) The line indicated by an asterisk has a bad shape; it was not used in the fit and does not occur in Table II. Three lines originating in the  $v_t = 0$  state are labeled below the spectrum, namely  $A$  and  $E$  components of the  $21_3-20_3$  transition (the strong doublet) and a  $b$ -type  $22_1-21_0 E$  transition. Many of the unassigned lines remaining in the spectrum are believed to originate in  $v_t = 3$  or 4.

First, the size of the torsional basis set retained after diagonalization of the purely torsional Hamiltonian (1-3, 7, 8) was increased from five functions to seven. This was necessary to achieve sufficient accuracy in calculated levels for  $v_t = 2$ .

Second, a somewhat arbitrary scheme was used to label and locate eigenvalues, since the more obvious scheme of simply using quantum numbers corresponding to the basis set function with the largest coefficient in a given eigenvector did not lead to unambiguous labeling results (9). Instead (10), a value for  $v_t$  was determined for each eigenvector by examining sums of coefficients for all basis set functions in that eigenvector with a given  $v_t$ . The  $K$  quantum number was then determined simply by the energy-ordering of the eigenvalues for each  $v_t$ . This empirical scheme leads to series of energy levels of fixed  $K$  and increasing  $J$  which are well described by power series in  $J(J+1)$ .

Third, a number of new terms were added to the Hamiltonian in the program, essentially to account for higher-order torsion-rotation interactions.

#### 4. RESULTS

After some trial and error, a satisfactory global fit of almost all microwave and infrared transitions involving  $v_t = 0, 1$ , and 2 torsional levels was obtained using 48 adjustable parameters. This number is somewhat less than the 53 parameters (i.e., 3 rotational constants and 5 centrifugal distortion constants for each of the six torsion-vibration levels plus 5  $\nu_0$  values) which might be used in a separate band-by-band analysis of the  $A$  and  $E$  components of  $v_t = 0, 1$ , and 2 torsional states.

Values for these parameters obtained from the global fit, as well as expressions for the corresponding operators, are given in Table I. The operators are grouped into sets labeled by the three integers  $n, l, m$  (11), where  $n \equiv l + m$  indicates the order (used for classifying terms in the Hamiltonian) of the total operator,  $l$  indicates the order of the torsional factor, and  $m$  indicates the order of the rotational factor. In order to fit these three torsional states, 7 parameters of order  $n = 2$ , 25 parameters of order  $n = 4$ , and 16 parameters of order  $n = 6$ , were used. These 48 parameters represent an increase of 14 over the  $34 = 7 (n = 2) + 22 (n = 4) + 5 (n = 6)$  parameters needed for the  $v_t = 0$  and 1 global fit (3), which is not surprising in view of the fact that the  $A$  and  $E$  components of one more torsional state are included in the present fit compared to that of Ref. (3) and the maximum value of  $J$  is almost doubled.

Table II gives assignments, observed frequencies, and observed minus calculated values from the fit for the new  $v_t = 0, 1$ , and 2 Nizhny Novgorod submillimeter measurements. Table III gives similar information for the new  $v_t = 2 \leftarrow 1$  far-infrared transitions. Tables I and II of Ref. (4) give the new millimeter-wave measurements of that work, with observed minus calculated values obtained from the present fit. Analogous tables for other measurements used in the fit are not given, since the quality of the fit here is very similar to that shown in Table II of Ref. (2), or Tables III and IV of Ref. (3).

The overall quality of the present fit is shown in Table IV, which gives the unitless (weighted) rms deviations for transitions grouped according to their measurement uncertainty (weight in the fit). Comparison of Table IV with similar information in Table III of Ref. (2) and Table V of Ref. (3) shows only modest deterioration in the quality of the fit for measurements treated previously.

TABLE I

The 48 Torsion-Rotation Parameters Used in the Present Global Fit of Transitions Involving Levels of the  $v_t = 0, 1$ , and 2 Torsional States of Acetaldehyde

$n\ell m^a$	Operator <sup>b</sup>	Parameter <sup>b</sup>	Value <sup>c</sup>	$n\ell m^a$	Operator <sup>b</sup>	Parameter <sup>b</sup>	Value <sup>c</sup>
220	$(1/2)(1-\cos 3\gamma)$	$V_3$	407.947(2)	404	$-P^4$	$\Delta_J$	$0.3212(3) \times 10^{-6}$
	$P_Y^2$	$F$	7.6559(6)		$-P_a^2 P_a^2$	$\Delta_{JK}$	$-0.28(1) \times 10^{-5}$
211	$P_Y P_a$	$\rho$	0.3291(2)		$-P_a^4$	$\Delta_K$	$0.1246(2) \times 10^{-3}$
202	$P_a^2$	$A$	1.8848741(9)		$-2P^2(P_b^2 - P_c^2)$	$\delta_J$	$0.750(1) \times 10^{-7}$
	$P_b^2$	$B$	0.3487163(5)		$-\{P_a^2, (P_b^2 - P_c^2)\}$	$\delta_K$	$0.223(5) \times 10^{-5}$
	$P_c^2$	$C$	0.3031777(1)		$(P_a P_b + P_b P_a) P^2$	$D_{abJ}$	$0.886(6) \times 10^{-6}$
	$(P_a P_b + P_b P_a)$	$D_{ab}$	-0.122709(3)		$(P_a^3 P_b + P_b P_a^3)$	$D_{abK}$	$0.213(7) \times 10^{-4}$
440	$P_Y^4$	$k_4$	$-0.4313(2) \times 10^{-3}$	642	$(1-\cos 6\gamma) P^2$	$N_v$	$0.479(2) \times 10^{-4}$
	$(1/2)(1-\cos 6\gamma)$	$V_6$	-12.918(8)		$(1-\cos 6\gamma) P_a^2$	$K_2$	$-0.279(4) \times 10^{-3}$
	$\{(1-\cos 3\gamma), P_Y^2\}$	$k_7$	-0.0445(3)		$P_Y^4 P^2$	$M_v$	$0.2(1) \times 10^{-8}$
431	$P_Y^3 P_a$	$k_3$	$-0.8363(4) \times 10^{-3}$		$2P_Y^4 (P_b^2 - P_c^2)$	$c_3$	$-0.15(6) \times 10^{-8}$
	$\{(1-\cos 3\gamma), P_Y P_a\}$	$k_6$	-0.033(2)	633	$P_Y^3 P_a P^2$	$k_{3J}$	$-0.22(2) \times 10^{-7}$
422	$P_Y^2 P^2$	$G_v$	$-0.284(3) \times 10^{-5}$	624	$P_Y^2 P_a^4$	$g_v$	$0.5(1) \times 10^{-10}$
	$P_Y^2 P_a^2$	$k_2$	$-0.9838(6) \times 10^{-3}$		$P_Y^2 P_a^2 P^2$	$k_{2J}$	$-0.25(1) \times 10^{-7}$
	$2P_Y^2 (P_b^2 - P_c^2)^d$	$c_1$	$-0.142(3) \times 10^{-5}$		$P_Y^2 P_a^4$	$k_{2K}$	$0.87(4) \times 10^{-7}$
	$P_Y^2 (P_a P_b + P_b P_a)$	$\Delta_{ab}$	$0.42(1) \times 10^{-4}$		$2P_Y^2 (P_b^2 - P_c^2) P^2$	$c_{1J}$	$-0.95(5) \times 10^{-10}$
	$\sin 3\gamma (P_a P_c + P_c P_a)$	$D_{ac}$	$-0.14(1) \times 10^{-2}$		$(1-\cos 3\gamma) P^4$	$f_v$	$-0.87(3) \times 10^{-8}$
	$(1-\cos 3\gamma) P^2$	$F_v$	$0.5587(4) \times 10^{-3}$		$(1-\cos 3\gamma) P_a^2 P^2$	$k_{5J}$	$0.28(9) \times 10^{-7}$
	$(1-\cos 3\gamma) P_a^2$	$k_5$	-0.031(1)		$(1-\cos 3\gamma) P_a^4$	$f_k$	$0.80(9) \times 10^{-6}$
	$(1-\cos 3\gamma) (P_b^2 - P_c^2)$	$c_2$	$0.2053(5) \times 10^{-3}$	615	$P_Y P_a^5$	$l_k$	$0.67(3) \times 10^{-7}$
	$(1-\cos 3\gamma) (P_a P_b + P_b P_a)$	$d_{ab}$	$0.2103(3) \times 10^{-2}$		$P_Y P_a^3 P^2$	$\lambda_v$	$-0.113(4) \times 10^{-7}$
413	$P_Y P_a P^2$	$L_v$	$0.60(1) \times 10^{-5}$	606	$P_a^4 P^2$	$H_{KJ}$	$-0.198(8) \times 10^{-8}$
	$P_Y P_a^3$	$k_1$	$-0.5596(3) \times 10^{-3}$		$P_a^6$	$H_K$	$0.113(7) \times 10^{-7}$
	$P_Y (P_a, \{P_b^2 - P_c^2\})$	$c_4$	$-0.429(8) \times 10^{-5}$				
	$P_Y (P_a^2 P_b + P_b P_a^2)$	$\delta_{ab}$	$0.60(2) \times 10^{-4}$				

<sup>a</sup>Notation of Ref. (11):  $n \equiv \ell + m$ , where  $n$  is the total order of the operator,  $\ell$  is the order of the torsional part and  $m$  is the order of the rotational part, respectively.

<sup>b</sup>Notation of Refs. (7,8).  $\{A, B\} \equiv AB + BA$ . The product of the parameter and operator from a given row yields the term actually used in the vibration-rotation-torsion Hamiltonian, except for  $F$ ,  $\rho$  and  $A$ , which occur in the Hamiltonian in the form  $F(P_Y + \rho P_a)^2 + AP_a^2$ .

<sup>c</sup>Values of the parameters from the fit shown in Tables II, III and IV. All values are in  $\text{cm}^{-1}$ , except for  $\rho$ , which is unitless. Uncertainties are shown as one standard deviation in the last digit.

<sup>d</sup>Note that a factor of 2 error in the  $c_1$  operator in Table II of Ref. (3) is corrected here.

## 5. DISCUSSION

The present fit of 3108 transitions to 48 parameters is excellent, particularly since we have included data from  $v_t = 0, 1$ , and 2 (i.e., from all torsional levels below the top of the internal rotation barrier) with  $J$  values up to 26 and  $K$  values up to 13. It should be noted, however, that  $\Delta K = 0$  rotational intervals within  $v_t = 2$  are determined experimentally only to  $\pm 1$  MHz by the RAD-3 submillimeter measurements, while  $\Delta K \neq 0$  rotational intervals are determined only to  $\pm 15$  MHz by the infrared hot band measurements. (No submillimeter  $v_t = 2$   $b$ -type lines are included in the fit, since  $b$ -

TABLE II

Assignments.<sup>a</sup> Observed  $\nu_i = 0, 1$ , and 2 Submillimeter Transitions.<sup>b</sup> and Observed Minus Calculated Values<sup>c</sup> from the Global Fit with Parameters Given in Table I and Weighted Root-Mean-Square Residuals Given in Table IV

$\nu_i$	J'	K <sub>a</sub> '	K <sub>b</sub> ' <sup>1</sup>	J''	K <sub>a</sub> ''	K <sub>b</sub> '' <sup>1</sup>	Obs <sup>b</sup>	O-C <sup>c</sup>	$\nu_i$	J'	K <sub>a</sub> '	K <sub>b</sub> ' <sup>1</sup>	J''	K <sub>a</sub> ''	K <sub>b</sub> '' <sup>1</sup>	Obs <sup>b</sup>	O-C <sup>c</sup>	$\nu_i$	J'	K <sub>a</sub> '	K <sub>b</sub> ' <sup>1</sup>	J''	K <sub>a</sub> ''	K <sub>b</sub> '' <sup>1</sup>	Obs <sup>b</sup>	O-C <sup>c</sup>	
2	9	2	7	8	2	6	165734.6	2.0	0	19	1	18	19	0	19	1	18	-0.1	2	7	1	7	6	0	6	219205.4	0.4
2	9	0	8	1	0	8	166689.5	1.6	2	10	5	5	9	5	4	194531.3	1.6	1	13	3	11	13	2	12	2	219756.9	0.6
2	9	5	4	8	5	3	167370.3	0.3	0	19	3	16	19	2	17	194758.5	0.4	2	11	1	10	10	1	9	219780.2	0.6	
0	7	5	5	8	5	4	167370.3	0.3	2	10	7	3	9	7	2	194983.9	0.5	1	19	2	18	19	1	19	220865.3	-0.2	
0	7	1	7	6	0	6	167542.2	-0.3	2	10	7	4	9	7	3	194983.9	0.5	2	11	0	11	10	10	10	221215.8	0.0	
1	17	1	16	17	0	17	167955.2	-0.1	0	25	2	23	25	1	24	195531.3	1.8	0	12	2	10	12	10	12	221831.1	0.0	
1	13	1	12	12	2	11	168192.5	-0.5	2	10	4	7	9	4	6	195617.9	0.2	1	11	2	9	11	11	11	222091.1	0.4	
1	13	2	12	13	1	13	168220.7	-1.3	2	10	2	8	9	2	7	195639.6	0.2	0	4	2	2	3	1	3	222150.2	0.4	
2	9	2	8	8	2	7	168939.1	1.1	2	10	7	4	9	7	3	195738.7	-1.6	0	4	2	2	3	1	3	222227.0	0.0	
2	9	3	6	8	3	5	169272.7	1.4	1	14	2	13	14	1	14	195803.0	0.0	1	14	3	12	14	2	13	222276.2	-1.0	
2	9	1	9	8	1	8	169374.2	-0.4	0	14	3	11	14	2	12	196003.4	0.7	0	21	1	20	21	1	21	222500.8	0.7	
0	23	2	21	23	1	22	170094.0	0.5	2	10	9	1	9	0	1	196821.3	-0.6	2	12	8	4	11	8	1	232073.6	-1.0	
2	9	6	3	8	6	2	170143.0	0.9	2	10	9	2	9	9	1	196821.3	-0.6	0	21	1	20	21	1	21	232284.9	-0.1	
2	9	6	4	8	6	3	170143.0	0.9	2	10	6	5	9	6	4	196967.9	-1.0	2	12	5	7	11	5	6	232986.8	0.4	
0	10	2	10	10	1	10	170292.4	-0.7	1	11	1	18	10	0	19	198002.2	-0.6	2	12	5	8	11	5	7	232986.8	0.3	
0	23	2	21	23	1	22	170411.1	-0.4	0	18	1	15	18	1	16	198371.4	-1.0	2	12	10	10	12	9	9	232924.0	0.0	
2	9	7	2	8	7	1	170983.0	-1.4	2	10	5	6	9	5	5	198818.0	0.4	0	17	2	16	17	1	17	224563.0	-0.4	
2	9	4	5	8	4	4	171576.4	0.1	1	2	2	0	1	1	0	199137.9	0.3	0	11	3	9	11	2	9	224878.5	0.7	
2	9	4	6	8	4	5	171576.4	0.4	0	18	3	15	18	2	16	199332.3	0.4	1	16	3	13	16	2	14	224951.8	0.2	
2	9	3	7	8	3	6	173220.6	-0.7	0	20	2	18	19	1	18	200547.3	-2.1	1	15	3	13	15	3	14	225220.2	0.0	
1	9	8	1	8	0	8	173137.3	-0.4	0	11	3	17	12	2	12	201193.5	-0.1	2	12	1	12	11	1	11	225166.9	-0.6	
1	9	8	2	8	1	7	173317.3	-0.4	0	3	2	1	2	1	2	201288.3	-1.0	2	12	3	9	11	3	8	225512.9	1.5	
2	9	1	8	8	1	7	173877.8	1.3	2	10	10	9	9	0	9	201479.1	-0.6	2	12	9	3	11	9	2	225630.0	0.1	
1	9	7	3	8	7	2	174002.4	0.8	1	19	2	17	18	3	16	202408.7	0.0	0	21	1	20	21	0	21	225740.9	0.5	
2	9	3	7	8	3	6	174177.8	-0.2	1	20	3	17	20	2	18	202859.8	-0.8	2	12	1	12	11	1	11	225737.7	-1.0	
2	9	2	8	8	2	7	174207.4	-0.7	0	17	3	15	17	2	15	203048.5	-0.5	0	17	2	16	17	1	17	225787.0	0.0	
2	9	2	8	8	2	7	174568.2	0.1	2	6	1	6	5	0	5	203720.9	-0.1	0	13	0	13	12	1	12	226487.7	0.5	
0	9	2	7	8	2	6	174982.6	0.1	0	15	1	14	14	2	13	203892.5	-0.4	2	12	6	6	11	6	5	226787.9	1.2	
2	9	5	4	8	5	3	175065.6	-1.0	0	17	3	14	17	2	15	204042.2	0.4	2	12	6	7	11	6	6	226787.9	1.2	
0	9	2	7	8	2	6	175090.8	0.1	2	11	8	3	10	8	2	204226.8	0.3	2	12	2	11	11	2	10	226981.2	0.6	
2	9	8	0	8	0	8	175211.3	-0.7	0	11	9	8	10	8	8	205167.7	0.8	2	12	8	10	12	7	9	230598.8	-0.4	
2	9	7	2	8	7	1	175742.8	1.1	0	15	1	14	14	2	13	204713.1	1.7	1	17	2	16	17	1	17	227631.1	-1.0	
2	9	7	3	8	7	2	175742.8	1.1	2	11	5	6	10	5	5	205066.1	0.0	2	12	7	5	11	7	4	228071.0	-0.4	
1	20	3	17	20	2	18	175762.8	0.3	2	11	5	7	10	5	6	205066.1	0.1	1	16	3	14	16	2	15	228816.9	-0.6	
1	14	2	13	14	1	13	175779.4	0.5	1	15	2	14	15	1	15	206097.6	0.6	1	16	2	18	16	3	17	229337.7	-0.4	
2	9	7	2	8	7	1	175841.3	-0.9	1	1	2	1	2	1	2	206097.6	-0.4	2	12	9	3	11	9	2	228935.6	-1.5	
1	3	2	2	3	1	2	175931.8	-1.7	0	20	1	19	20	1	20	206114.9	-2.3	2	12	4	9	11	4	8	228935.6	-0.8	
2	9	7	3	8	7	2	176135.1	-0.2	0	15	2	14	15	1	15	206373.9	-0.6	1	15	3	12	15	2	13	229030.2	0.3	
2	9	6	4	8	6	3	177194.0	-0.6	2	11	3	8	10	3	7	206715.3	-0.9	0	16	1	15	15	1	14	230187.1	1.7	
2	9	8	1	8	0	8	177450.8	-0.5	2	11	1	11	10	1	10	206823.2	-1.6	1	12	0	12	11	0	11	230187.1	1.7	
2	9	8	2	8	1	7	177450.8	-0.5	0	11	2	10	11	1	10	206890.7	-0.1	2	12	1	10	11	1	10	230461.6	0.1	
0	18	1	17	18	0	18	177813.5	0.7	2	11	1	11	10	1	10	207518.3	0.7	0	5	2	4	4	1	3	230601.0	-0.2	
2	9	4	5	8	4	4	178156.5	1.2	0	15	2	14	15	1	15	207595.8	-0.3	1	12	10	2	11	10	1	230757.2	0.2	
0	14	1	13	14	1	13	178436.6	-0.2	2	11	2	10	12	9	8	207703.8	-0.3	1	12	10	3	11	10	2	230757.2	0.2	
0	18	1	17	18	0	18	178497.7	0.1	16	3	15	16	2	14	207712.4	0.8	1	12	9	11	12	9	11	230757.2	0.2		
0	2	2	2	3	1	2	178497.7	0.1	16	3	15	16	2	14	207712.4	0.8	1	12	9	11	12	9	11	230757.2	0.2		
2	9	5	5	8	5	4	178949.4	0.9	0	16	3	13	16	2	14	208730.6	0.5	2	12	10	2	11	10	1	232365.2	0.8	
0	25	3	22	25	2	23	178975.5	0.9	2	11	7	4	10	7	3	209034.8	0.2	2	12	3	9	11	3	8	232474.7	0.3	
0	24	3	21	24	2	22	179240.4	0.2	1	7	3	6	7	2	5	209353.0	0.1	2	12	2	11	11	2	10	232504.1	0.3	
0	14	1	13	14	1	13	179311.2	-0.2	1	16	1	15	16	1	15	209365.0	0.7	1	12	7	4	9	11	2	232504.1	0.3	
0	2	2	2	3	1	2	179712.1	-0.5	0	26	2	24	26	1	25	209742.8	2.2	2	12	7	6	11	7	5	232745.5	1.4	
0	24	3	21	24	2	22	179781.6	0.4	2	11	4	7	10	4	6	209803.2	-0.3	2	12	5	7	11	5	6	233530.1	0.5	
0	26	3	23	26	2	24	179883.0	0.7	2	11	4	8	10	4	7	209803.2	1.0	2	12	8	5	11	8	4	233745.8	0.2	
2	9	1	8	8	1	7	180020.3	0.6	1	5	3	2	5	2	3	210055.1	-1.5	2	12	4	8	11	4	7	234739.9	0.7	
2	9	3	20	23	2	21	180510.6	-0.2	1	3	3	2	3	1	2	210517.0	-0.8	2	12	10	2	11	10	1	234962.0	-0.6	
0	2	2	2	3	1	2	180795.2	-0.4	1	4	3	1	4	2	2	210647.0	-1.2	2	12	10	2	11	10	1	235291.4	-0.6	
0	23	3	20	23	2	21	181195.5	0.2	0	10	5	6	11	4	7	210222.3	-1.4	2	12	10	3	11	10	2	235291.4	-0.6	
2	9	0	9	8	0	8	181480.7	0.0	0	20	1	19	20	0	20	210222.3	0.5	2	12	10	3	11	10	2	235458.1	0.3	
0	24	2	22	24	1	23	182196.7	1.0	1	4	3	2	4	2	3	210428.0	1.5	0	18	2	17	18	1	18			

TABLE II—Continued

$v_L$	$J_K$	$K'_L$	$J'_K$	$K''_L$	$K''_L''$	Obs	O-C	$v_L$	$J'_K$	$K'_L$	$K'_L''$	$J''_K$	$K''_L$	$K''_L''$	Obs	O-C	$v_L$	$J'_K$	$K'_L$	$K'_L''$	$J''_K$	$K''_L$	$K''_L''$	Obs	O-C	
2	13	-13	-11	12	-3	10	249597.3	0.4	0	15	0	15	14	0	14	281127.2	0.3	2	16	-8	8	15	-8	7	298917.3	0.8
1	13	-12	-2	12	-12	1	249807.5	0.7	1	15	0	15	14	0	14	282023.5	0.0	0	16	0	16	15	0	15	299077.7	0.2
1	13	10	3	12	10	2	249989.3	0.0	2	15	0	15	14	3	11	282284.7	0.6	0	16	0	16	15	0	15	299174.3	-0.5
1	13	10	3	12	10	2	250000.0	0.0	0	15	0	15	14	3	11	282300.0	0.0	0	16	0	16	15	0	15	299181.0	0.0
1	13	9	4	-12	9	3	250032.8	0.3	1	18	-1	17	-17	2	16	282954.5	0.1	0	23	4	19	23	3	20	299911.7	-0.2
1	13	9	5	12	9	4	250032.8	0.3	2	15	6	9	14	6	8	283509.6	0.7	2	16	1	16	15	1	15	300001.1	-0.1
1	13	7	6	12	7	5	250159.5	0.2	2	15	6	10	14	9	8	283509.6	0.8	2	16	5	11	15	5	10	300077.7	0.3
1	13	6	7	12	6	6	250159.5	0.2	2	15	6	10	14	9	8	283509.6	0.8	2	16	5	11	15	5	10	300077.7	0.3
1	13	5	8	12	5	7	250308.3	0.9	2	15	10	10	14	10	10	284352.2	-0.2	0	16	0	16	15	0	15	30017.3	-0.6
1	13	8	6	-12	8	5	250388.3	0.9	2	15	2	13	14	2	12	285446.2	-1.1	2	16	3	13	15	3	12	301352.1	-1.5
1	13	-6	8	12	-6	7	251061.8	0.8	2	15	0	15	14	0	14	286190.1	-0.8	1	19	4	15	19	3	16	301852.7	-2.0
1	13	-9	5	12	-9	4	251199.4	0.7	0	15	-3	13	14	1	11	286821.1	-0.7	2	16	6	10	15	6	9	302447.0	0.8
2	13	7	7	12	7	7	251300.0	0.0	0	15	0	15	14	0	14	287000.0	0.0	0	16	0	16	15	0	15	302644.5	0.0
2	13	-10	3	12	-10	2	251301.1	1.4	0	6	5	1	7	4	4	287651.2	-0.5	2	16	-2	15	-2	15	-2	303101.4	0.8
1	13	-8	6	12	-8	5	251388.8	0.6	0	6	5	2	7	4	3	287651.2	-0.2	2	16	10	7	15	10	6	303142.2	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	251419.0	0.1	0	16	0	16	15	1	15	288004.7	0.9	1	18	4	14	18	3	15	304165.5	-0.1
2	13	12	-1	12	12	0	25																			

TABLE II—Continued

$v_t$	$J'$	$K_a'$	$K_c'$	$P'$	$J''$	$K_a''$	$K_c''$	$P''$	$Obs^b$	O-C <sup>c</sup>	$v_t$	$J'$	$K_a'$	$K_c'$	$P'$	$J''$	$K_a''$	$K_c''$	$P''$	$Obs^b$	O-C <sup>c</sup>	$v_t$	$J'$	$K_a'$	$K_c'$	$P'$	$J''$	$K_a''$	$K_c''$	$P''$	$Obs^b$	O-C <sup>c</sup>
0	8	2	6	+	7	1	7	+	314392.4	1.0	2	17	4	13	16	4	12	328342.1	-0.7	1	12	4	9	12	3	10	345477.7	-0.6				
2	16	-4	13	15	-4	12	314582.1	0.1	2	17	-4	14	16	-4	13	328362.0	0.1	2	18	-10	8	17	-10	7	10	345633.9	-0.1					
0	25	-2	24	25	-1	25	314633.4	0.0	0	18	4	15	-18	3	16	328409.0	-1.6	1	18	-13	6	17	-13	5	345850.8	0.8						
1	18	-4	14	18	-3	15	314710.8	0.0	0	13	4	10	-13	3	11	328520.3	-0.6	1	18	-12	7	17	-12	6	346020.6	0.5						
1	16	2	14	15	2	13	314755.0	0.0	0	2	17	2	16	2	15	328564.5	-0.7	1	18	2	17	17	2	16	346064.9	-0.4						
0	16	2	14	15	2	13	314934.5	0.3	1	17	-14	16	-3	13	328645.9	-0.6	1	18	10	8	17	10	7	+	346161.1	0.5						
0	16	2	14	15	2	13	314957.5	0.2	0	19	4	16	-19	3	17	328675.8	-0.4	1	18	10	9	17	10	8	+	346161.1	0.5					
2	16	0	16	15	0	15	315074.8	1.3	1	17	-17	11	16	-7	10	328675.8	0.2	1	18	9	9	17	9	8	+	346270.2	0.8					
2	17	11	7	16	11	6	315381.7	1.7	1	17	6	11	16	4	10	328714.4	-0.5	1	18	9	10	17	9	9	+	346270.2	0.8					
0	17	-1	17	16	-1	16	315628.3	0.3	0	2	17	12	-16	6	11	328714.4	-0.4	2	18	7	11	17	7	10	+	346459.9	-0.3					
0	17	1	17	16	1	16	315645.5	0.1	1	17	-8	10	16	-8	9	328739.0	-0.1	1	18	11	7	17	11	6	+	346509.2	-0.1					
2	16	6	11	15	6	10	315752.1	0.6	1	17	4	14	16	4	13	328775.5	0.1	1	18	11	8	17	11	7	+	346509.2	-0.1					
1	17	-4	13	17	-3	14	315816.8	0.1	0	11	4	8	-11	3	9	328797.2	-1.2	0	18	13	5	17	13	4	+	346653.1	1.0					
2	16	2	14	15	2	13	315890.5	0.9	0	9	4	5	+	3	6	328955.5	-1.4	0	18	13	6	17	13	5	+	346653.1	1.0					
1	17	1	17	16	1	14	315998.6	0.4	1	17	15	16	3	14	15	329151.6	-0.4	0	18	12	7	17	12	6	+	346672.2	0.6					
1	17	1	17	16	1	16	316649.3	0.1	0	20	4	17	-20	3	18	329110.4	-0.3	0	18	11	7	17	11	6	+	346756.6	0.7					
1	21	4	18	-21	3	19	316926.2	0.3	0	8	4	5	-8	3	6	329131.4	-0.4	0	18	11	8	17	11	7	+	346756.6	0.7					
1	17	0	17	16	0	16	317231.4	0.1	0	7	4	4	+	3	5	329206.7	-0.9	0	18	-11	7	17	-11	6	+	346756.6	2.1					
0	17	0	17	16	0	16	317249.6	-0.1	0	6	4	3	+	3	4	329248.8	2.4	0	18	9	10	17	9	9	+	348006.4	-1.5					
0	17	0	17	16	0	16	317292.0	0.2	0	4	4	0	+	4	3	329322.3	-1.4	0	18	10	8	17	10	7	+	348006.4	1.0					
2	17	-1	17	16	-1	16	317590.4	1.0	0	4	4	1	-4	3	2	329322.3	-2.7	0	18	10	9	17	10	8	+	348006.4	1.0					
2	17	-8	9	16	-8	8	317971.8	0.4	2	17	13	15	16	3	14	329354.6	-0.2	0	18	9	9	17	9	8	+	348084.1	-0.9					
1	13	-4	9	13	-3	10	318172.7	1.2	1	17	4	14	16	4	13	329410.5	-0.2	0	18	9	10	17	9	9	+	348084.1	-0.9					
1	17	0	17	16	0	16	318302.1	0.2	1	17	4	13	16	12	+	329550.7	-0.3	0	18	8	10	17	8	9	+	348893.4	-0.3					
2	16	1	15	15	1	14	318500.2	0.7	0	11	18	-11	21	3	13	318500.2	-0.7	0	18	11	7	17	11	6	+	348893.4	-0.3					
1	12	-4	8	12	-3	9	318544.4	0.6	0	17	3	14	16	3	13	330228.5	0.4	0	18	8	11	17	8	10	+	348893.4	-0.3					
1	22	4	19	-22	3	20	318506.9	1.6	0	17	3	14	16	3	13	330243.9	-0.2	0	18	-7	11	17	-7	10	+	349094.3	0.1					
2	17	1	17	16	1	16	318554.9	0.3	1	17	1	16	-1	15	+	330580.6	0.1	0	18	7	11	17	7	10	+	349657.4	-0.1					
1	10	-4	6	10	-3	7	318807.8	0.2	0	22	4	19	-22	3	20	330633.8	-1.2	0	18	12	+	17	12	11	+	349657.4	-0.1					
1	17	1	16	15	1	14	318906.5	0.1	0	20	19	-20	2	18	+	330696.7	0.2	0	18	7	12	17	7	11	+	349697.0	0.5					
1	5	-4	1	5	-3	2	319011.9	0.9	1	20	-1	19	19	2	18	330776.4	0.3	0	18	6	12	17	6	11	+	347071.6	0.0					
1	6	-4	2	6	-3	3	319011.9	-0.8	1	17	3	14	-16	3	13	331038.9	-0.3	0	18	6	13	17	6	12	+	347071.6	0.0					
2	17	5	12	-16	5	11	319184.9	0.0	0	20	1	19	19	-2	18	331202.7	0.2	0	18	2	18	20	-1	20	+	347071.6	0.2					
2	17	5	12	-16	5	11	319184.9	0.0	0	20	1	19	19	-2	18	331202.7	0.2	0	18	2	18	20	-1	20	+	347071.6	0.2					
0	18	4	14	18	3	15	319385.1	0.0	0	17	8	10	16	8	9	331342.4	0.0	1	18	-14	17	-14	13	+	347181.9	-0.5						
2	17	3	14	16	3	13	320574.3	0.5	0	17	1	16	-16	1	15	331602.5	0.4	1	18	5	13	17	5	12	+	347217.7	0.9					
2	17	6	11	16	6	10	321402.7	0.5	0	17	1	16	-16	1	15	331680.5	0.1	1	18	-5	14	17	-5	13	+	347252.2	0.3					
2	17	6	12	-16	6	11	321402.7	0.6	2	17	11	6	-16	11	5	331764.6	-0.1	1	18	9	9	17	9	8	+	347325.9	1.6					
0	17	4	13	17	3	14	321679.8	0.2	2	17	11	7	16	11	6	331764.6	-0.1	1	18	7	11	17	7	10	+	347325.9	1.6					
2	17	-2	16	16	-2	15	321843.2	0.5	0	23	4	20	-23	3	21	331799.4	0.6	1	18	7	12	17	7	11	+	347459.6	0.3					
2	17	10	8	16	10	7	322140.6	-0.3	1	17	-1	16	-16	-1	15	332214.0	0.1	0	18	3	16	17	3	15	+	347519.4	0.3					
1	17	1	17	16	0	16	323215.8	-0.1	1	25	1	15	14	0	14	332253.2	-1.4	0	18	-3	16	17	-3	15	+	347563.6	0.3					
2	17	-7	10	16	-7	9	324401.4	0.5	2	17	0	17	16	0	16	332927.1	0.9	0	18	-4	15	17	-4	14	+	347756.8	0.6					
1	16	4	12	16	3	11	325371.7	0.0	2	17	7	11	16	7	10	333304.6	0.7	1	18	10	8	17	10	7	+	347795.7	1.0					
1	4	3	2	4	3	2	324039.8	-0.7	2	17	8	9	16	8	8	333419.5	0.3	1	18	11	7	17	11	6	+	347957.7	1.0					
0	11	2	10	-10	1	9	324627.5	-0.2	2	17	8	10	-16	8	9	333419.5	0.5	1	18	-7	12	17	-7	11	+	348010.3	-0.3					
0	17	-1	17	16	0	16	324772.9	-0.5	1	17	-2	15	16	-2	14	333473.3	0.2	1	18	6	12	17	6	11	+	348087.5	-0.5					
2	17	4	14	-16	4	13	324806.7	0.3	2	17	-13	6	-16	-11	5	333608.1	-1.9	1	18	6	13	17	6	12	+	350445.9	0.2					
0	17	4	13	16	3	15	324846.3	0.2	1	18	1	16	-17	1	17	333957.0	0.0	1	18	6	11	17	6	10	+	348087.5	-0.4					
0	17	3	17	16	2	15	324947.4	-0.1	0	18	1	18	17	1	17	333957.0	0.0	1	18	3	16	17	3	15	+	348211.6	0.7					
0	17	-2	16	16	-2	15	324977.1	-0.3	1	22	4	19	22	3	20	334251.9	0.3	1	18	4	15	17	4	14	+	348229.1	-0.4					
0	17	2	16	16	2	15	324996.3	-0.8	1	18	1	18	17	1	17	334341.5	0.1	1	18	-3	15	17	-3	14	+	348288.5	-0.1					
1	17	2	16	16	2	15	325038.7	-0.8	1	17	2	15	16	2	14	334637.4	0.0	2	18	3	16	17	3	15	+	348748.7	-0.4					
2	17	1	16	16	1	15	325273.5	0.0	2	17	7	11	16	7	10	334904.6	0.2	1	18	4	14	17	4	13	+	349062.3	-0.3					
2	17	-1	15	16	-1	14	326617.3	-0.5	0	17	2	15	16	2	14	334904.6	0.1	1	18	4	14	17	4	13	+	349062.3	-0.3					
1	17	-1	13	15	-1	12	326633.9	-0.2	0	17	2	15	16	2	14	334931.8	0.4	1	18	1	17	17	1	16	+	349320.2	-0.2					
1	17	1	17	16	0	16	326728.5	-1.0	1	18	1	18	17	1	17	334981.2	0.4	1	18	2	13	17	2	12								

TABLE II—Continued

$v_t$	$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$P''$	Obs <sup>b</sup>	O-CC	$v_t$	$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$P''$	Obs <sup>b</sup>	O-CC	$v_t$	$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$P''$	Obs <sup>b</sup>	O-CC
2	19	3	16	18	3	15		359798.2	-0.1	1	15	2	14	14	-1	13		371056.9	-0.9	0	20	4	17	-19	4	16	-	386454.5	-0.7
1	19	1	19	18	0	18		360290.3	1.1	0	7	3	4	-	2	5		371082.2	-0.1	0	20	-4	17	-19	-4	16	-	386543.0	0.4
2	19	10	10	18	10	9		360379.4	-1.8	2	19	2	17	18	2	16		371392.7	0.0	1	20	-7	14	-19	-7	13	-	386678.4	-0.2
2	19	1	18	18	1	17		361317.8	-0.6	0	20	0	20	19	0	19		371492.4	0.4	1	20	-3	18	-19	3	17	-	386731.7	0.1
2	19	-7	12	18	-7	11		361608.3	-0.9	0	20	0	20	-19	0	19		371496.1	0.2	1	20	-8	13	-18	-8	12	-	386748.5	0.4
1	6	4	5	2	4			362425.8	0.4	1	20	1	20	19	1	19		371596.4	0.2	0	20	4	16	-19	4	15	-	386866.8	0.3
0	19	-2	18	18	-2	17		362534.7	0.4	1	20	0	20	-19	0	19		371695.1	0.4	1	20	4	17	-19	4	16	-	387193.6	-0.1
0	19	2	18	18	2	17		362561.1	-0.3	2	19	8	11	-18	8	10		371962.5	-0.8	1	20	5	16	-19	5	15	-	387429.7	0.3
1	19	2	18	18	2	17		362579.9	-0.5	2	19	8	11	-18	8	11		371912.5	-0.2	1	20	5	15	-19	5	14	-	387447.4	-0.4
2	19	4	16	18	4	15		362647.8	-0.4	1	20	0	20	19	0	19		372636.7	-0.2	0	20	1	19	-19	1	18	-	387483.0	0.2
2	19	4	15	18	4	14		363315.9	0.0	2	19	7	13	18	7	12		372771.7	0.9	2	20	3	18	-19	3	17	-	387504.4	-0.6
0	14	-2	13	13	1	12		363566.6	0.0	2	19	10	9	-18	10	8		372842.2	0.8	0	20	1	19	-19	1	18	-	387573.5	0.1
1	8	3	6	7	2	5		363985.9	1.8	2	19	10	10	-18	10	9		372842.2	-1.1	1	20	4	17	-19	4	16	-	387753.5	-0.3
0	14	2	13	-13	1	12		364495.8	-0.2	2	20	-1	20	-19	-1	19		372893.6	0.8	1	20	-3	17	-19	-3	16	-	387968.2	0.1
2	19	-10	9	18	-10	8		364514.6	-0.9	2	20	11	10	19	11	9		373287.9	0.2	0	21	-3	19	-20	3	17	-	388084.3	1.5
1	19	2	18	18	2	17		364565.7	-0.9	2	19	-11	8	-18	-11	7		373518.3	-6.5	1	20	4	16	-19	4	15	-	388173.5	-0.4
1	19	-13	7	18	-13	6		365067.1	1.5	1	19	-2	17	18	-2	16		373899.4	0.1	0	8	3	6	-7	2	5	-	388378.5	-0.8
1	19	-12	8	18	-12	7		365264.7	0.6	2	20	1	20	-19	1	19		373536.3	0.5	1	20	-1	19	-19	-1	18	-	388523.6	-0.4
1	19	10	9	18	10	9		365306.1	-1.0	1	19	-7	17	-18	-6	16		374205.6	0.4	2	20	3	18	-19	3	17	-	388568.2	-0.3
1	19	10	10	18	10	9		365396.1	-1.0	2	19	5	15	18	5	14		374226.3	0.3	0	16	-15	15	1	14	-	388654.2	-0.2	
1	19	9	10	18	9	9		365523.7	0.3	0	19	2	17	18	2	16		374645.7	0.2	0	21	-1	21	-20	-1	20	-	388753.2	0.0
1	19	9	11	18	9	10		365573.7	0.3	0	19	2	17	-18	2	16		374682.4	0.7	0	21	1	21	-20	1	20	-	388773.5	-0.2
1	19	7	12	18	7	11		365573.1	0.1	1	20	1	20	-19	0	19		375041.5	-0.7	2	20	3	17	-19	3	16	-	389146.5	0.6
1	19	11	8	18	11	7		365745.9	0.6	2	19	6	14	18	6	13		375121.2	0.7	1	21	1	21	-20	1	20	-	389259.3	-0.3
1	19	11	9	18	11	8		365745.9	0.6	2	19	6	14	18	-4	15		375142.1	1.4	0	21	0	21	-20	0	20	-	389543.8	-0.5
0	19	13	6	18	13	5		365899.2	-0.6	2	20	-8	12	-18	-8	11		375292.0	-0.9	0	21	0	21	-20	0	20	-	389578.6	-0.6
0	19	13	7	18	13	6		365899.2	-0.6	0	20	-8	12	-19	0	19		375494.6	0.1	1	21	0	21	-20	0	20	-	389585.3	-0.6
0	19	11	9	18	11	8		366013.2	-0.5	2	20	-7	14	-18	-7	13		375737.8	-0.1	1	21	0	21	-20	1	20	-	390080.1	-0.8
0	19	12	7	18	12	6		365954.0	-0.6	1	7	-3	4	-	2	4		376243.0	0.7	1	17	16	-16	-1	15	-	390210.1	-1.2	
0	19	12	8	18	12	7		365954.0	-0.6	2	19	2	17	-18	2	16		376629.0	0.7	0	20	3	17	-19	3	16	-	390165.5	0.5
0	19	-13	6	18	-13	5		365971.7	0.0	2	19	1	18	-18	1	17		376679.7	-0.2	0	20	3	17	-19	3	16	-	390183.7	-0.2
0	19	11	8	18	11	7		366013.2	-0.5	0	15	2	14	-14	1	13		377115.9	-1.5	2	20	11	9	-19	11	8	-	390431.0	-0.2
0	19	11	9	18	11	8		366013.2	-0.5	2	20	-2	19	-18	-2	18		377372.8	-1.3	2	20	11	10	-19	11	9	-	390531.0	-0.2
0	19	-11	8	18	-11	7		366013.2	-1.9	2	20	0	20	-19	0	19		377558.3	0.7	0	8	3	5	-7	2	6	-	390710.4	0.0
1	19	8	11	18	8	10		366037.7	-0.4	2	20	6	14	-19	6	13		378398.4	-0.2	1	21	0	21	-20	0	20	-	390753.9	0.3
0	19	10	9	18	10	8		366069.4	0.1	2	20	6	15	-19	6	14		378398.4	0.1	1	20	3	17	-19	3	16	-	390951.0	1.2
0	19	10	10	18	10	9		366069.4	0.1	1	22	-1	21	-21	2	20		378571.1	0.4	2	20	2	18	-19	2	17	-	390951.0	-2.1
1	19	8	11	18	8	10		366078.8	0.2	2	20	10	11	-19	10	9		378737.8	-1.3	2	20	8	12	-19	8	11	-	391078.8	-0.6
1	19	8	12	18	8	11		366069.4	0.8	0	22	-1	21	-21	2	20		379632.2	0.2	2	20	8	13	-19	8	12	-	391079.8	-0.5
0	19	9	10	18	9	9		366119.6	-0.6	0	22	1	21	-21	2	20		380009.9	0.9	2	21	-1	21	-20	-1	20	-	391316.1	0.7
0	19	9	11	18	9	10		366119.6	-0.6	2	20	1	19	-19	1	18		380034.7	0.1	2	20	7	14	-19	7	13	-	392434.9	0.9
0	19	-8	11	18	-8	10		366119.6	1.8	2	20	3	17	-19	3	16		382043.1	-0.1	2	21	1	21	-20	1	20	-	392503.4	0.7
0	19	8	11	18	8	10		366174.8	0.2	2	20	-7	13	-18	-7	12		380730.9	0.2	2	20	10	10	-19	10	9	-	392521.8	-0.2
0	19	8	12	18	8	11		366174.8	0.9	0	20	-2	19	-18	-2	18		381242.9	1.6	2	20	10	11	-19	10	10	-	392521.8	0.9
0	19	8	12	18	8	11		366174.8	0.2	1	7	3	5	-6	2	5		381519.5	0.3	1	21	1	21	-20	0	20	-	392607.0	0.1
0	19	-7	12	18	-7	11		366229.7	0.7	2	20	4	17	-19	4	16		382485.9	0.3	2	21	11	11	-20	11	10	-	392689.1	-0.2
0	19	7	12	18	7	11		366252.6	0.1	1	20	4	16	-18	4	15		382583.8	-0.3	0	21	1	21	-20	0	20	-	392786.7	0.1
0	19	7	13	18	7	12		366252.6	-0.1	1	20	5	19	-18	5	18		382643.3	-0.3	1	21	1	21	-20	1	20	-	392807.0	0.1
0	19	7	13	18	7	12		366293.3	0.3	2	20	-10	10	-19	10	9		383424.8	-0.1	1	13	-12	11	-12	-11	11	-	393190.9	0.1
0	19	6	13	18	6	12		366389.9	0.1	1	20	-13	8	-18	-13	7		384281.2	0.4	2	20	5	16	-19	5	15	-	393270.2	-0.5
0	19	6	14	18	6	13		366389.9	0.4	1	20	-12	9	-18	-12	8		384499.3	0.6	1	20	2	18	-19	2	17	-	393871.0	-0.2
0	19	-6	13	18	-6	12		366411.3	0.9	1	20	10	10	-19	10	9		384634.3	-0.1	1	20	-2	18	-19	-2	17	-	393936.9	-0.1
0	19	6	14	18	6	13		366456.2	0.2	2	20	10	11	-19	10	10		384634.3	-0.1	1	20	-2	18	-19	-2	17	-	393936.9	-0.1
0	20	0	20	-19	-1	19		366470.5	0.0	2	20	7	13	-19	7	12		384723.5	-1.2	0	20	2	18	-19	2	17	-	394433.2	0.4
1	19	13	6	18	13	5		366505.4	0.1	2	20	7	14	-19	7	13		384723.5	-1.1	1	21								



TABLE II—Continued

$v_t$	$J'$	$K_A'$	$K_C'$	$P'$	$J''$	$K_A''$	$K_C''$	$P''$	Obs <sup>b</sup>	$0-C^c$	$v_t$	$J'$	$K_A'$	$K_C'$	$P'$	$J''$	$K_A''$	$K_C''$	$P''$	Obs <sup>b</sup>	$0-C^c$	$v_t$	$J'$	$K_A'$	$K_C'$	$P'$	$J''$	$K_A''$	$K_C''$	$P''$	Obs <sup>b</sup>	$0-C^c$	
0	22	6	22	+21	1	21	+	404369.8	1.0	0	21	4	18	-20	4	17	-	405865.5	0.3	0	21	3	18	-20	3	17	-	410317.4	0.4				
0	22	0	22	21	-1	21		404393.7	-0.9	1	21	3	19	+20	3	18	+	405908.7	-0.1	1	21	3	18	-20	3	17	-	411040.8	0.0				
0	21	12	10	20	12	9		404423.2	0.1	0	21	1	20	-20	1	19	-	405942.1	-0.3	0	25	5	20	-25	4	21	+	411102.8	1.3				
1	21	6	15	20	6	14		404510.8	0.7	0	21	4	18	-20	4	17	-	405942.1	0.8	1	22	22	21	0	21		42002.3	0.4					
0	21	10	12	20	10	11		404525.7	0.2	1	21	-7	15	-20	-7	14		406012.5	-0.4	2	22	11	12	21	11	11		412118.7	-1.0				
0	21	11	10	-20	11	9		404525.7	-0.4	1	21	-8	14	-20	-8	13		406062.9	0.0	2	21	7	15	-20	7	14		412158.3	1.9				
0	21	11	11	+20	11	10	+	404525.7	-0.4	1	21	6	15	+20	6	14	+	406242.1	-0.2	2	21	10	11	+20	10	10	+	412214.0	0.2				
0	21	-10	11	-20	-10	10		404547.3	0.3	1	21	6	16	-20	6	15	-	406242.1	0.6	2	21	10	12	-20	10	11	-	412214.0	2.3				
1	21	8	13	20	8	12		404564.1	-0.6	0	21	4	17	+20	4	16	+	406408.7	-0.1	2	21	5	17	-20	5	16	-	412253.3	0.2				
0	21	9	13	20	9	12		404620.0	0.3	0	21	4	17	-20	4	16		406443.7	0.4	0	18	-2	17	17	1	16		413098.0	-0.4				
0	21	9	12	-20	9	11		404631.5	0.1	0	9	3	7	+	8	2	6	+	406632.0	-0.1	0	24	5	19	-24	4	20	+	413196.6	0.8			
0	21	9	13	+20	9	12	+	404653.5	0.1	1	21	4	18	-20	4	17	-	406659.1	-0.2	1	21	5	16	-21	4	17	+	413348.8	1.2				
0	21	-8	13	20	-8	12		404680.6	0.3	1	21	5	17	+20	5	16	+	406870.3	0.0	1	21	2	19	+20	2	18	+	413448.2	0.4				
0	21	8	13	+20	8	12	+	404741.3	0.9	1	21	5	16	-20	5	15	-	406898.8	0.0	2	22	-8	14	-21	-8	13	+	413597.8	0.1				
0	21	8	14	20	8	13		404741.3	-0.6	0	22	-1	22	-21	-1	21		406988.3	0.3	2	22	0	22	+21	0	21	+	413807.8	0.3				
0	21	8	14	-20	8	13		404741.3	0.9	0	22	1	22	+21	1	21	+	407009.1	0.2	1	21	-2	19	-20	-2	18	-	413829.7	-0.1				
2	21	2	20	-20	2	19	-	404763.2	-0.9	1	21	-1	20	-20	-1	19	-	407022.6	-0.5	2	22	-2	21	-21	-2	20	-	413861.0	0.1				
0	21	-7	14	-20	-7	13		404829.0	0.0	1	21	4	18	-20	4	17	-	407202.9	0.7	0	21	2	19	-20	2	18	-	414038.3	-0.3				
0	21	7	14	+20	7	13	+	404851.7	-0.4	1	22	1	22	+21	1	21	+	407355.5	0.4	0	21	2	19	+20	2	18	+	414085.8	-0.4				
0	21	7	15	+20	7	14	+	404851.7	-0.4	1	21	5	1	+	4	3	2	+	407568.6	-1.7	1	18	2	17	17	-1	16		414189.6	-0.4			
6	21	7	15	-20	6	14		404898.1	0.1	1	5	4	-2	-4	3	1	-	407568.6	-0.1	1	20	5	15	-20	4	16	+	414230.6	-0.4				
0	21	6	15	+20	6	14	+	405044.1	-0.2	6	22	0	22	21	0	21		407634.9	0.0	2	21	6	16	-20	6	15	-	414539.2	0.7				
0	21	6	16	-20	6	15	-	405044.1	-0.6	6	22	0	22	+21	0	21	+	407667.7	-0.2	0	23	5	18	-23	4	19	+	414448.3	2.0				
0	21	-6	15	-20	-6	14		405069.2	0.0	1	1	23	4	17	+20	4	16	+	407782.0	-0.2	0	23	-3	21	-22	3	19	-	415208.8	4.6			
0	21	6	16	20	6	15		405114.8	0.2	1	21	3	19	-20	3	18		407796.8	-0.5	1	5	-4	1	-4	-3	1		415239.1	0.8				
1	21	9	12	-20	9	11		405162.0	-0.2	1	22	0	22	+21	0	21	+	408018.6	-0.2	1	20	5	16	+20	4	17	-	415484.0	-0.4				
1	21	-10	12	-20	-10	11		405172.7	0.2	1	23	-3	18	-20	-3	17	-	408087.6	0.4	1	19	5	15	-19	4	16	-	415808.2	-0.6				
0	21	3	19	+20	3	18	+	405225.9	0.4	1	22	1	22	21	1	21		408151.4	-0.2	0	22	5	17	-22	4	18	-	416402.0	-0.2				
0	21	-3	19	-20	-3	18		405246.0	0.7	0	26	5	21	-26	4	22	+	408609.0	-2.0	1	16	5	11	-16	4	12	+	416430.7	0.6				
1	21	-5	16	-20	-5	15		405283.3	-0.6	1	22	5	22	-21	0	21		408877.5	0.2	2	22	6	16	+21	6	15	+	416516.8	-0.7				
1	21	5	16	20	5	15		405360.3	-0.4	2	21	3	18	-20	3	17	-	408931.1	1.1	1	22	6	17	-21	6	16	-	416516.8	0.3				
0	21	5	17	+20	5	16	+	405388.4	0.1	2	21	8	14	-20	8	13		409545.3	1.5	1	15	5	10	-15	4	11	+	416747.8	-0.4				
0	21	5	16	-20	5	15	-	405445.0	-0.1	2	22	-1	22	-21	-1	21		409727.2	1.4	0	26	5	22	+26	4	23	+	416784.7	0.8				
0	21	5	17	-20	5	16		405466.0	-0.7	2	21	-5	16	-20	-5	15		409845.8	1.4	1	15	5	11	-15	4	12	-	416887.1	-0.6				
0	21	-5	16	-20	-5	15		405466.0	-1.7	2	21	8	13	+20	8	12	+	410201.9	-2.4	1	14	5	9	-14	4	10	+	417002.7	-0.8				
1	21	7	14	-20	7	13		405466.0	-0.1	2	21	8	14	-20	8	13		410201.9	-0.6	2	21	2	19	-20	2	18	+	417085.1	1.5				
1	21	7	15	+20	7	14	+	405466.0	-0.1	0	22	-1	22	-21	0	21		410228.5	0.3	1	13	5	8	-13	4	9	+	417205.8	-1.0				
1	21	-9	13	-20	-9	12		405787.6	0.4	0	21	3	18	-20	3	17	-	410295.1	0.7	0	25	5	21	+25	4	22	+	417240.6	0.7				
0	21	1	20	20	1	19		405849.4	0.2																								

in Nizhny Novgorod to measure selected  $a$ -type and  $b$ -type transitions (predicted from the present fit), but such measurements are significantly more time consuming than the broadband RAD-3 measurements, and the great increase in precision will undoubtedly require some improvement in the model as well.

Comparison of values of parameters from the present fit with those obtained in our earlier fit of the lower- $J$ ,  $v_t = 0$  and 1 data (3) shows that the main rotational parameters  $A$ ,  $B$ ,  $C$  change by about 0.01%, while the principal torsional parameters  $V_3$ ,  $F$ ,  $\rho$  change by about 1%. Values for some of the higher-order parameters, however, differ greatly from the values obtained in Ref. (3). All of the parameters in our fit are "effective" parameters, containing unknown contributions from vibrational averaging effects, etc. Differences between values obtained from the  $v_t = 0$ , 1 and  $v_t = 0$ , 1, 2 fits thus give a measure of the model errors in the present formalism. It will be interesting to see how stable these parameters remain when  $v_t = 3$  and 4 data are added to the fit.

The parameters obtained from our global  $v_t = 0$ , 1, 2, fit can be used to calculate pure torsional ( $J = K = 0$ )  $A$  species energy levels at 75.3570, 219.1004, and 330.5813  $\text{cm}^{-1}$  for  $v_t = 0$ , 1, and 2, respectively, and analogous pure torsional  $E$  species levels at 75.4260, 217.3505, and 344.4691  $\text{cm}^{-1}$ , where the zero of energy corresponds to the minimum of the internal rotation potential well.

A number of local perturbations were observed in the calculated  $v_t = 2$  levels, particularly for both  $A$  and  $E$  species levels with  $K = 9$ . (Many transitions involving these perturbed levels have not actually been located at the present time.) Preliminary calculations of levels belonging to  $v_t = 3$  and 4 suggest that perturbation of the  $v_t = 2$ ,  $K = -9$   $E$  levels arises from  $v_t = 3$ ,  $K = -4$  levels, but this conclusion has not been confirmed. Complete analysis of such perturbations, which appear to originate completely within the torsional manifold, must await analysis of the  $v_t = 3$  and 4 torsional levels.

TABLE III

Assignments, <sup>a</sup> Observed  $\nu_i = 2 \leftarrow 1$  Far-Infrared Transitions, <sup>b</sup> and Observed Minus Calculated Values<sup>c</sup> from the Global  $\nu_i = 0, 1$ , and 2 Fit with Parameters Given in Table I and Weighted Root-Mean-Square Residuals Given in Table IV

J' K <sub>a</sub> ' K <sub>c</sub> ' P'	J'' K <sub>a</sub> '' K <sub>c</sub> '' P''	Obs <sup>b</sup>	0-C <sup>c</sup>	J' K <sub>a</sub> ' K <sub>c</sub> ' P'	J'' K <sub>a</sub> '' K <sub>c</sub> '' P''	Obs <sup>b</sup>	0-C <sup>c</sup>	J' K <sub>a</sub> ' K <sub>c</sub> ' P'	J'' K <sub>a</sub> '' K <sub>c</sub> '' P''	Obs <sup>b</sup>	0-C <sup>c</sup>
12 11 2 + 12 10 2 +	148.7236	-0.0004	24 7 18 + 23 6 18 -	156.0489	-0.0001	17 1 17 + 17 0 17 +	114.3831	-0.0005			
12 11 1 + 12 10 1 +	148.7236	-0.0004	25 7 19 + 24 6 18 -	156.0586	-0.0001	18 1 18 + 18 0 18 +	114.4130	-0.0006			
13 11 3 + 13 10 3 +	148.8463	-0.0011	26 7 20 + 25 6 20 -	157.0228	-0.0005	19 1 19 + 19 0 19 +	114.4430	-0.0007			
13 11 2 + 13 10 2 +	148.8463	-0.0011	11 6 5 + 11 5 7 +	144.4665	0.0005	4 1 3 - 3 0 3 -	117.6365	0.0003			
15 11 5 + 15 10 5 +	149.1176	0.0003	11 6 6 + 11 5 6 -	144.4665	0.0005	5 1 4 - 4 0 4 -	118.4183	0.0003			
15 11 4 + 15 10 4 +	149.1176	0.0003	13 6 7 + 13 5 9 +	144.0907	0.0007	6 1 5 - 5 0 5 -	119.2314	-0.0004			
17 11 7 + 17 10 7 +	149.4297	-0.0002	13 6 8 + 13 5 8 -	144.0907	0.0007	7 1 6 + 6 0 6 +	119.2201	-0.0007			
17 11 6 + 17 10 6 +	149.4297	-0.0002	17 6 11 + 17 5 13 +	143.1470	-0.0010	2 0 2 + 2 1 2 +	110.2660	-0.0010			
11 11 1 + 10 10 0 +	155.6683	0.0001	17 6 12 + 17 5 12 -	143.1470	-0.0007	4 0 4 + 4 1 4 +	110.4261	-0.0005			
11 11 0 + 10 10 0 +	155.6683	0.0001	11 6 5 + 10 5 5 -	151.5642	-0.0003	5 0 5 + 5 1 5 +	110.5380	-0.0006			
12 11 2 + 11 10 1 +	156.4215	0.0003	11 6 6 + 10 5 6 -	151.5642	-0.0003	6 0 6 + 6 1 6 +	110.6704	-0.0003			
12 11 1 + 11 10 0 +	156.4215	0.0003	12 6 6 + 11 5 6 -	152.0305	-0.0003	7 0 7 + 7 1 7 +	110.8213	-0.0003			
13 11 3 + 12 10 3 +	157.1838	-0.0002	12 6 7 + 11 5 7 -	152.0305	-0.0003	8 0 8 + 8 1 8 +	110.9893	-0.0004			
13 11 2 + 12 10 2 +	157.1838	-0.0002	14 6 8 + 13 5 8 -	152.9156	-0.0001	11 0 11 + 11 1 11 +	111.5791	-0.0004			
14 11 4 + 13 10 4 +	157.9560	-0.0006	14 6 9 + 13 5 9 -	152.9156	-0.0001	12 0 12 + 12 1 12 +	111.7972	-0.0001			
14 11 3 + 13 10 3 +	157.9560	-0.0006	16 6 10 + 15 5 10 -	153.7390	0.0006	13 0 13 + 13 1 13 +	112.0218	-0.0003			
16 11 6 + 15 10 6 +	159.5320	0.0001	16 6 11 + 15 5 11 -	153.7390	0.0005	15 0 15 + 15 1 15 +	112.4829	-0.0003			
16 11 5 + 15 10 5 +	159.5320	0.0001	6 15 + 20 5 15 -	155.5420	0.0002	16 0 16 + 16 1 16 +	112.7153	-0.0001			
17 11 7 + 16 10 7 +	160.3350	0.0001	11 5 6 + 10 4 6 +	153.1088	0.0005	17 0 17 + 17 1 17 +	112.9460	-0.0003			
17 11 6 + 16 10 6 +	160.3350	0.0001	11 5 7 + 10 4 7 +	153.1088	0.0003	18 0 18 + 18 1 18 +	113.1741	-0.0004			
18 11 8 + 17 10 8 +	161.1494	0.0009	13 5 8 + 12 4 8 +	153.8344	0.0013	19 0 19 + 19 1 19 +	113.3989	0.0000			
18 11 7 + 17 10 7 +	161.1494	0.0009	14 5 8 + 13 4 8 +	153.8344	0.0013	20 0 20 + 20 1 20 +	113.6183	-0.0001			
19 11 9 + 18 10 9 +	161.9726	-0.0001	17 5 12 + 16 4 12 +	155.1244	0.0008	21 0 21 + 21 1 21 +	113.8300	-0.0002			
19 11 8 + 18 10 8 +	161.9726	-0.0001	17 5 13 + 16 4 13 +	155.1244	0.0008	22 0 22 + 22 1 22 +	114.0419	-0.0005			
20 11 10 + 19 10 10 +	162.8077	0.0000	12 5 7 + 12 4 7 -	145.7303	0.0003	1 0 3 + 1 1 3 +	107.5109	0.0000			
20 11 9 + 19 10 9 +	162.8077	0.0000	12 5 8 + 12 4 8 -	145.7303	0.0001	4 0 4 + 4 1 4 +	106.8153	-0.0004			
21 11 11 + 20 10 11 +	163.6540	0.0002	13 5 8 + 13 4 8 -	145.7303	0.0004	5 0 5 + 5 1 5 +	107.1099	-0.0005			
21 11 10 + 20 10 10 +	163.6540	0.0002	13 5 9 + 13 4 9 -	145.7303	0.0004	6 0 6 + 6 1 6 +	107.3938	0.0000			
23 11 13 + 22 10 13 +	165.3800	0.0002	6 4 2 + 6 3 4 -	143.1607	0.0008	7 0 7 + 7 1 7 +	104.6641	-0.0012			
12 10 2 + 12 9 1 +	141.4900	0.0000	4 4 3 - 3 3 4 -	143.1607	0.0014	6 1 6 + 6 2 4 +	109.1885	0.0004			
12 10 1 + 12 9 0 +	141.4900	0.0000	12 4 8 + 12 3 10 -	142.6421	0.0002	1 2 2 + 4 2 2 +	107.1000	-0.0004			
14 10 4 + 13 9 4 +	141.8293	-0.0002	14 4 10 + 13 3 12 +	142.6421	0.0004	4 1 3 + 5 1 3 +	106.5074	-0.0005			
14 10 3 + 13 9 3 +	141.8293	-0.0002	15 4 12 + 15 3 12 -	142.1528	0.0005	5 1 4 - 6 2 4 -	106.0111	-0.0006			
10 10 0 + 9 9 0 +	147.6174	-0.0002	17 4 13 + 17 3 15 +	142.0000	-0.0004	1 3 3 + 4 2 3 -	106.8711	-0.0009			
10 10 1 + 9 9 1 +	147.6174	-0.0002	19 4 16 + 19 3 16 -	141.2715	0.0006	4 1 4 + 5 2 4 +	106.1723	-0.0008			
11 10 1 + 10 9 0 +	148.3564	-0.0001	20 4 17 + 20 3 17 -	140.9882	-0.0003	6 1 6 + 7 2 6 +	108.7351	-0.0002			
11 10 0 + 10 9 0 +	148.3564	-0.0001	6 4 3 - 5 3 4 -	147.0290	0.0009	3 1 2 - 3 2 2 -	109.6807	-0.0008			
12 10 2 + 11 9 1 +	149.1882	-0.0002	11 4 7 + 10 3 7 -	149.8363	0.0010	4 1 3 - 4 2 3 -	109.7839	0.0008			
12 10 1 + 11 9 0 +	149.1882	-0.0002	12 4 8 + 11 3 8 -	150.3664	0.0014	6 1 5 - 6 2 5 -	110.0628	-0.0001			
13 10 4 + 12 9 4 +	149.9931	-0.0003	12 4 9 + 11 3 9 -	150.3666	0.0007	2 2 1 - 3 3 1 +	110.1668	-0.0008			
13 10 3 + 12 9 3 +	149.9931	-0.0003	14 4 10 + 13 3 12 +	150.3666	0.0007	3 2 2 + 4 3 2 +	111.0050	-0.0003			
14 10 5 + 13 9 5 +	150.8114	-0.0002	19 4 16 + 18 3 16 -	153.9841	0.0013	8 2 7 - 9 3 7 -	106.3860	-0.0001			
15 10 5 + 14 9 5 +	151.6428	-0.0003	20 4 16 + 19 3 16 -	154.0404	0.0015	2 2 0 + 3 3 0 -	110.1668	-0.0012			
15 10 4 + 14 9 4 +	151.6428	-0.0003	8 3 6 + 8 2 6 -	173.6032	0.0011	2 2 1 + 4 3 1 +	109.5336	-0.0011			
16 10 6 + 15 9 6 +	155.1050	0.0004	10 3 8 + 10 2 8 -	133.5197	0.0005	4 2 2 + 5 3 2 +	108.3038	-0.0004			
16 10 5 + 15 9 5 +	155.1050	0.0004	9 3 8 + 9 2 8 -	133.5197	0.0005	5 2 2 + 6 3 2 +	107.2559	-0.0005			
22 10 12 + 21 9 12 +	157.8509	-0.0003	11 3 9 + 11 2 9 -	133.4528	0.0005	3 3 0 - 4 4 0 -	113.6839	0.0002			
24 10 14 + 23 9 14 +	159.7589	-0.0009	12 3 10 + 12 2 10 -	133.3671	0.0002	4 3 1 - 5 4 1 -	113.0393	0.0002			
12 9 4 + 11 8 4 +	145.7132	-0.0001	12 3 9 + 12 2 11 -	133.9402	0.0005	5 3 2 - 6 4 2 +	112.3950	0.0005			
12 9 3 + 11 8 3 +	145.7132	-0.0001	13 3 11 + 13 2 11 +	133.2626	0.0002	6 3 3 - 7 4 3 +	111.7003	0.0002			
13 9 5 + 12 8 5 +	146.5398	-0.0003	13 3 12 + 13 2 12 +	133.1388	0.0003	8 3 5 - 9 4 5 -	110.4613	-0.0002			
13 9 4 + 12 8 4 +	146.5398	-0.0003	14 3 12 + 14 2 12 +	133.1388	0.0003	9 3 6 - 10 4 6 -	109.8171	-0.0005			
16 9 8 + 15 8 8 +	149.1113	-0.0009	16 3 14 + 16 2 14 +	132.8357	-0.0002	6 4 2 + 6 5 2 +	118.8509	0.0010			
16 9 7 + 15 8 7 +	149.1113	-0.0009	13 3 14 + 13 2 14 -	134.3912	-0.0002	7 4 3 + 8 5 3 +	118.4364	-0.0006			
18 8 10 + 17 7 10 +	138.1201	-0.0005	18 3 16 + 18 2 16 +	132.4701	0.0008	10 4 6 + 10 5 6 +	118.5350	0.0012			
18 8 9 + 17 7 9 +	138.1201	-0.0005	6 3 4 + 5 2 4 -	137.5175	0.0003	11 4 8 + 11 5 8 +	118.4344	0.0008			
12 8 4 + 11 7 4 +	146.0010	-0.0001	6 3 3 + 5 2 3 -	137.5161	0.0004	11 4 7 + 11 5 7 +	118.4344	0.0008			
13 8 5 + 12 7 5 +	146.8046	-0.0007	10 3 8 + 9 2 8 -	140.5244	0.0014	12 4 9 + 12 5 9 +	118.3261	0.0008			
13 8 4 + 12 7 4 +	146.8046	-0.0007	7 3 8 + 6 2 8 -	140.6298	0.0009	12 4 8 + 12 5 8 +	118.3261	0.0008			
16 8 8 + 15 7 8 +	149.2714	-0.0006	13 3 8 + 10 2 8 -	140.6298	0.0009	13 4 10 + 13 5 10 +	118.2102	0.0010			
16 8 7 + 15 7 7 +	149.2714	-0.0006	13 3 10 + 12 2 10 +	141.7812	-0.0004	13 4 9 + 13 5 9 +	118.2102	0.0006			
17 8 9 + 16 7 9 +	150.0930	0.0000	15 3 12 + 14 2 12 +	142.8705	-0.0001	14 4 11 + 14 5 11 +	118.0872	0.0016			
17 8 8 + 16 7 8 +	150.0930	0.0000	16 3 14 + 15 2 14 +	144.5461	0.0004	14 4 10 + 14 5 10 +	118.0872	0.0010			
18 8 10 + 17 7 10 +	150.9123	0.0001	17 3 15 + 16 2 15 -	145.3120	-0.0011	15 4 12 + 15 5 12 +	117.9577	0.0011			
18 8 9 + 17 7 9 +	150.9123	0.0001	19 3 16 + 18 2 16 +	144.9096	-0.0006	10 4 7 + 11 5 7 +	111.4364	0.0011			
19 8 11 + 18 7 11 +	151.7281	0.0001	21 3 19 + 20 2 19 -	148.6047	0.0006	11 4 7 + 12 5 7 +	110.6892	0.0003			
20 8 12 + 19 7 12 +	151.7281	0.0001	23 3 21 + 22 2 21 -	150.3798	0.0011	11 4 8 + 12 5 8 +	110.6892	0.0003			
20 8 11 + 19 7 11 +	152.5384	0.0002	5 2 3 + 5 1 5 -	123.4270	-0.0002	12 4 8 + 13 5 8 +	109.9353	0.0010			
20 8 10 + 19 7 10 +	152.5384	0.0002	6 2 4 + 6 1 6 -	123.5745	-0.0012	12 4 9 + 13 5 9 +	109.9353	0.0011			
11 7 5 + 11 6 5 +	141.0866	0.0000	7 2 5 + 7 1 7 -	123.7540	-0.0017	13 4 9 + 14 5 9 +	109.1722	0.0005			
11 7 4 + 11 6 4 +	141.0866	0.0000	7 2 6 + 7 1 6 -	122.8055	-0.0002	13 4 10 + 14 5 10 +	109.1722	0.0008			
13 7 7 + 13 6 7 +	141.1668	0.0002	8 2 6 + 8 1 8 -	123.9697	-0.0003	14 4 10 + 15 5 10 +	108.4015	0.0001			
13 7 6 + 13 6 6 +	141.1668	0.0002	9 2 7 + 9 1 9 -	124.2230	0.0012	14 4 11 + 15 5 11 +	108.4015	0.0006			
17 7 12 + 16 6 12 +	141.1402	-0.0003	10 2 8 + 10 1 10 -	124.5154	0.0008	15 4 12 + 16 5 12 +	107.6243	0.0015			
18 7 13 + 17 6 13 +	141.1402	-0.0003	10 2 9 + 10 1 11 -	122.5674	-0.0001	15 4 11 + 16 5 11 +	107.6243	0.0007			
19 7 13 + 16 6 13 +	141.0866	-0.0004	11 2 9 + 11 1 11 -	124.5154	0.0008	16 4 13 + 17 5 13 +	106.8387	0.0014			
19 7 12 + 16 6 12 +	141.0866	-0.0004	11 2 10 + 11 1 12 -	122.4779	-0.0011	10 5 6 + 11 6 6 +	107.7524	0.0008			
11 7 5 + 10 6 5 +	148.1776	0.0000	12 2 10 + 12 1 12 -	125.2370	-0.0002	10 5 5 + 11 6 5 +	107.7524	0.0008			
11 7 4 + 10 6 4 +	148.1776	0.0000	11 2 11 + 13 1 13 -	125.6741	-0.0001	11 5 7 + 12 6 7 +	106.8564	0.0008			
12 7 6 + 11 6 6 +	148.8676	-0.0001	14 2 13 + 14 1 13 -	122.2087	-0.0001	11 5 6 + 12 6 6 +	106.8564	0.0008			
12 7 5 + 11 6 5 +	148.8676	-0.0001	15 2 13 + 15 1 15 -	126.7144	-0.0003	10 6 4 + 11 7 4 +	99.1638	0.0002			
13 7 7 + 12 6 7 +	149.5482	-0.0001	6 2 4 + 5 1 5 -	128.8392	-0.0002	10 6 5 + 11 7 5 +	99.1638	0.0002			
13 7 6 + 12 6 6 +	149.5482	-0.0001	7 2 6 + 6 1 6 -	128.8392	-0.0002	12 6 6 + 13 7 6 +	97.5721	0.0002			
14 7 8 + 13 6 8 +	150.2173	-0.0001	8 2 7 + 7 1 7 -	129.0574	-0.0002	13 6 7 + 14 7 7 +	97.5721	0.0002			
14 7 7 + 13 6 7 +	150.2173	-0.0001	10 2 8 + 9 1 8 -	129.2952	-0.0001	11 6 7 + 14 7 7 +	96.7550	0.0000			
15 7 9 + 14 6 9 +	150.8733	-0.0002	11 2 9 + 10 1 9 -	129.9319	0.0005	13 6 8 + 14 7 8 +	96.7550	0.0000			
15 7 8 + 14 6 8 +											

TABLE III—Continued

$J^1 K_a^1 K_c^1 P^1$			$J^0 K_a^0 K_c^0 P^0$			Obs <sup>b</sup>	O-C <sup>c</sup>	$J^1 K_a^1 K_c^1 P^1$			$J^0 K_a^0 K_c^0 P^0$			Obs <sup>b</sup>	O-C <sup>c</sup>					
14	8	7	13	7	6	149.8911	0.0007	9	3	6	9	2	8	135.0996	-0.0004	123.9771	0.0001			
15	8	8	14	7	7	150.6532	-0.0001	11	3	8	11	2	10	134.6595	-0.0003	8	-3	5	124.0522	-0.0011
11	7	5	11	6	5	133.0360	0.0004	12	3	9	12	2	11	134.4084	0.0000	9	-4	9	124.1407	0.0003
12	7	6	12	6	6	133.1706	-0.0003	17	3	14	17	2	16	133.1226	-0.0003	12	-4	9	124.4726	-0.0004
13	7	7	13	6	7	133.3181	-0.0006	6	3	3	5	2	4	139.4353	-0.0002	13	-4	10	124.6081	-0.0006
14	7	8	14	6	8	133.4789	-0.0003	11	1	10	11	0	11	134.7663	-0.0005	16	-4	11	125.1090	-0.0003
17	7	11	17	6	11	134.0195	-0.0004	6	1	5	5	0	5	138.2167	-0.0001	17	-4	14	125.3094	-0.0006
12	6	3	12	5	7	129.6185	-0.0010	8	1	7	7	0	7	139.5593	0.0003	18	-4	15	125.5290	0.0001
13	6	8	13	5	8	129.6104	-0.0008	9	1	8	8	0	8	140.2581	0.0002	19	-4	16	125.7493	-0.0003
14	6	9	14	5	9	129.8190	-0.0005	4	-3	2	5	-4	1	97.5851	0.0004	6	-4	3	127.7626	-0.0009
16	6	11	16	5	11	130.2847	-0.0007	6	-3	4	7	-4	3	96.3380	0.0006	8	-4	5	129.1919	0.0000
17	6	12	17	5	12	130.5615	-0.0005	8	-3	6	9	-4	5	95.0668	-0.0008	9	-4	6	129.9233	-0.0005
18	6	13	18	5	13	130.8128	-0.0006	9	-3	7	10	-4	6	94.4221	-0.0001	10	-4	7	130.6653	-0.0007
20	6	15	20	5	15	131.3944	-0.0008	12	-3	10	13	-4	9	92.4412	-0.0011	11	-4	8	131.4201	-0.0007
11	6	10	10	5	5	136.3140	-0.0005	13	-3	11	14	-4	10	91.7686	-0.0007	12	-4	9	132.0722	-0.0003
12	6	7	11	5	6	137.1331	-0.0003	5	-1	5	5	-2	3	114.7097	0.0001	17	-4	10	136.7224	-0.0001
14	6	9	13	5	8	138.8209	-0.0006	7	-2	6	7	-1	6	117.7277	0.0001	18	-4	15	137.1464	-0.0002
16	6	11	15	5	10	140.5773	0.0006	8	-2	7	8	-1	7	117.4781	-0.0001	21	-4	18	139.8946	0.0000
17	6	12	16	5	11	141.4779	-0.0006	12	-2	11	12	-1	11	116.3556	-0.0010	22	-4	19	140.8439	-0.0003
19	6	14	18	5	13	143.3261	0.0000	13	-2	12	13	-1	12	116.0488	-0.0008	23	-4	20	141.8011	0.0001
20	6	15	19	5	14	144.2685	-0.0007	7	-2	6	6	-1	5	122.2982	-0.0007	11	-5	6	139.2452	0.0006
11	5	7	11	4	8	129.4806	-0.0010	8	-2	7	7	-1	6	122.7125	-0.0010	12	-5	7	139.9665	-0.0009
18	5	14	18	4	15	131.1254	-0.0010	14	-2	13	13	-1	12	124.8967	-0.0009	13	-5	8	140.6976	-0.0003
11	5	7	10	4	7	136.5659	-0.0007	17	-2	16	16	-1	15	125.8039	-0.0018	14	-5	9	141.4365	-0.0003
12	5	8	11	4	8	137.4332	-0.0007	11	-3	9	11	-2	9	119.3987	0.0014	15	-5	10	142.1819	0.0001
15	5	11	14	4	11	140.0871	-0.0009	12	-3	10	12	-2	10	119.3192	0.0000	17	-5	12	146.6971	-0.0002
16	5	12	15	4	12	140.9764	-0.0015	15	-3	13	15	-2	13	118.9213	-0.0005	18	-5	13	147.3804	-0.0001
18	5	14	17	4	14	142.7419	-0.0002	17	-3	15	17	-2	15	118.4961	-0.0008	15	-6	9	147.3804	0.0001
6	4	2	5	3	3	135.9752	-0.0012	19	-3	17	19	-2	17	117.9557	0.0008	16	-6	10	147.4052	0.0011
7	4	3	6	3	4	136.4716	-0.0009	20	-3	18	20	-2	18	117.6513	0.0010	11	-6	5	140.1740	0.0002
8	4	4	7	3	5	137.2640	-0.0006	7	-3	5	6	-2	4	124.0350	0.0009	13	-6	7	145.6987	0.0008
13	4	9	12	3	10	140.9882	0.0001	10	-3	8	9	-2	7	125.9087	0.0013	14	-6	8	151.3635	0.0008
14	4	10	13	3	11	141.6632	0.0005	12	-3	10	11	-2	9	127.0853	0.0006	15	-6	9	152.0505	0.0003
24	4	20	23	3	21	147.1833	0.0008	14	-3	12	13	-2	11	128.1819	0.0001	17	-6	11	153.3693	0.0001
7	3	4	7	2	6	135.4339	-0.0004	14	-3	15	16	-2	14	129.6205	0.0001					

It seems clear from the number of remaining unassigned submillimeter lines that numerous rotational transitions with  $v_t = 3$  are present in the Nizhny Novgorod spectrum, and it seems possible that transitions with  $v_t = 4$  will also be present with reasonable intensity. These torsional states are above the barrier, however, and we suspect that various approximations in the present theoretical model, which were introduced for the lower torsional levels, will have to be changed before levels above the barrier can be accurately calculated.

An additional theoretical problem needing investigation is the question of what approximate quantum numbers to use in place of  $K_a$  and  $K_c$  in order to obtain un-

TABLE IV  
Root-Mean-Square Deviations from the Global Fit of Tables I-III

Number of parameters			48		
RMS of the 1014 $v_t=0-0$ MW Lines			0.536 MHz		
RMS of the 840 $v_t=1-1$ MW Lines			0.519 MHz		
RMS of the 430 $v_t=2-2$ MW Lines			0.910 MHz		
RMS of the 420 $v_t=1-0$ FIR Lines			0.00039 cm <sup>-1</sup>		
RMS of the 404 $v_t=2-1$ FIR Lines			0.00060 cm <sup>-1</sup> <sup>a</sup>		

Lines <sup>b</sup>	Uncertainty <sup>c</sup>	RMS <sup>d</sup>	Lines <sup>b</sup>	Uncertainty <sup>c</sup>	RMS <sup>d</sup>
10	0.004-0.005	3.4	392	0.080	1.1
2	0.010	0.7	6	0.100	0.7
60	0.020	1.8	14	0.130-0.200	0.9
485	0.030-0.050	1.2	1315	1.0	0.8

<sup>a</sup>The far-infrared hot-band lines were given an uncertainty  $\sqrt{2}$  times larger than the  $v_t=1-0$  lines, i.e., an uncertainty of 0.00050 cm<sup>-1</sup>, to allow for expected but undetected blending with weak lines from the fundamental band.

<sup>b</sup>Number of MW lines in each uncertainty group.

<sup>c</sup>Experimental uncertainty range in MHz for each group.

<sup>d</sup>Dimensionless root-mean-square weighted deviation for each group, which should be unity if the fit is good to experimental uncertainty.

ambiguous and theoretically meaningful quantum number labels for the final eigenvectors. It is likely that this question is complicated by the fact that different approximate quantum numbers will be needed for the three limiting cases of torsional levels well below the top of the barrier, torsional levels at the top of the barrier, and torsional levels well above the top of the barrier.

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