

# GAUCHE ETHYL ALCOHOL: LABORATORY ASSIGNMENTS AND INTERSTELLAR IDENTIFICATION

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Received 1996 August 9; accepted 1996 November 7

## ABSTRACT

Ethyl alcohol (ethanol) is known to possess a pair of closely spaced excited torsional substates (gauche+, gauche−) at an energy of approximately 57 K above the ground (trans) torsional substate. We report an extended analysis of some gauche− → gauche+ *Q*-branch ( $\Delta J = 0$ ) transitions with a three-substate fixed frame axis method (FFAM) Hamiltonian. Our approach accounts for complex trans–gauche interactions for the first time. In addition, we are able to obtain intensities for perturbed rotational transitions, and to determine the trans to gauche+ separation to be 1185399.1 MHz. A complete ground state rotational-torsional partition function accounting for the previously neglected gauche substates is presented. Based on our analysis, a total of 14 *U* lines obtained towards Orion KL can now be assigned to gauche substates of ethanol. Analysis of these lines yields a rotational temperature of 223 K and a total (trans + gauche) column density of  $7.0 \times 10^{15} \text{ cm}^{-2}$ . The column density is in reasonable agreement with the recent value of  $2\text{--}3 \times 10^{15} \text{ cm}^{-2}$  based on observations of trans-ethanol by Ohishi et al., although there is some disparity in the rotational temperatures. Eight additional *U* lines in the literature are assigned to transitions of gauche ethanol.

*Subject headings:* ISM: molecules — line: identification — molecular data — molecular processes — radio lines: ISM

## 1. INTRODUCTION

Ethyl alcohol (ethanol) has been observed in several warm, dense interstellar clouds. It was initially detected in Sgr B2 by Zuckerman et al. (1975) and later detected in W51M by Millar et al. (1988) with a large fractional abundance of  $10^{-8}$ . Ethanol has also been reported towards Orion KL by Turner (1989, 1991) and (tentatively) by Ziurys & McGonagle (1993). The most recent detection towards Orion KL, and the most convincing, has been made by Ohishi et al. (1995). These authors detected four lines of ethanol and obtained a column density of  $\approx 1 \times 10^{15} \text{ cm}^{-2}$  and a rotational temperature of  $\approx 70$  K. Also, quite recently, a large number of submillimeter transitions have been detected in the Hot Core G34.3+0.15, and a rotational temperature of 125 K and a column density of  $2.0 \times 10^{15} \text{ cm}^{-2}$  derived (Millar, Macdonald, & Habing 1995). The recent observations suggest that ethanol is primarily localized in hot core regions with gas densities of  $10^6\text{--}10^8 \text{ cm}^{-3}$  and temperatures near or in excess of 100 K. Although several mechanisms for forming ethanol in the gas phase have been proposed (Millar et al. 1988), its large abundance in hot cores suggests a major role for dust chemistry (Charnley et al. 1995). In these sources, it is probable that ethanol or a suitable precursor was formed on the surfaces of dust particles during a previous colder era. Once star formation began, the regions warmed, evaporating the ethanol or precursor (Caselli, Hasegawa, & Herbst 1993).

The rotational spectrum of ethanol is complicated and often perturbed by internal rotation (torsional) motions,

especially by the motion of the hydroxyl (OH) proton, that lead to trans and gauche substates. In the ground vibrational state, the trans substate is the lowest in energy; rotational transitions in this substate are the ones previously observed in the interstellar medium. The rotational spectrum of ethanol has been the subject of many previous laboratory investigations; summaries are given in Pearson et al. (1995, 1996). In our first paper on the ground vibrational state spectrum of ethanol (Pearson et al. 1995), we measured and analyzed a large number of millimeter wave and submillimeter-wave rotational transitions in the trans substate, while in our second paper (Pearson et al. 1996) we measured and analyzed a large number of transitions in the two closely spaced gauche states (gauche+ and gauche−), which lie only 57 K above the trans substate and should be easily excited in warm interstellar regions (although no identifications of interstellar gauche-ethanol have been previously reported, to the best of our knowledge). The rotational transitions in the gauche substates consist of transitions within each substate and transitions which cross from one substate to the other.

Previous laboratory investigations of rotational transitions in the ground vibrational state of ethanol have treated the trans and two gauche substates as noninteracting, but such analyses are only successful for a limited range of the quantum numbers *J* and *K<sub>a</sub>* (Pearson et al. 1995, 1996) due to strong trans–gauche interactions outside this range. In this paper, we report the first combined trans- and gauche-ethanol ground state analysis, the precise trans to gauche energy difference, and laboratory spectra of four often perturbed *c*-type ( $\Delta K_a = \pm 1$ ,  $\Delta K_c = 0$ ) gauche− to gauche+ *Q*-branches ( $\Delta J = 0$ ) and their perturbation-allowed *x*-type ( $\Delta K_a = 0$ ,  $\Delta K_c = 0$ ) counterparts.

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Our previous analysis of gauche ethanol and our current combined trans-gauche analysis have enabled us to assign and analyze 14 *U* lines in the 97.5–98.0 GHz region as belonging to three different *Q*-branches between the gauche torsional substates of ethanol. The *U* lines were observed in Orion KL and reported by Ohishi et al. (1988) as part of a search for the PS radical. These transitions have line widths on the order of  $3 \text{ km s}^{-1}$ , consistent with a hot core source called the Compact Ridge that is known for its oxygen-rich organic molecules (Blake et al. 1987). Ohishi et al. (1988) speculated that the *U* lines were high-lying but ruled out methanol and its  $^{13}\text{C}$  isotopomer as the carriers. Although the majority of the *U* lines can be assigned directly from the results of Pearson et al. (1996), there are some which lie above the *J* and *K<sub>a</sub>* limits of that analysis. These lines show significant perturbations with the trans substate; as a result, line strength and transition frequency calculations require the model of the entire ground state presented in this paper. With intensities generated by our model, we can determine the ethanol column density and rotational temperature in Orion KL. We also propose assignments of eight other previously reported *U* lines to gauche ethanol *Q*-branch transitions.

## 2. THEORY

Ethanol is a prolate asymmetric top ( $\kappa \approx -0.92$ ) with two large-amplitude internal motions, the threefold internal rotation of the protons of the methyl group, and the asymmetric internal rotation of the hydroxyl proton. The methyl internal rotation has  $\text{C}_3$  group symmetry, which results in A and E substates with A to A and E to E selection rules. The

threefold symmetric ( $\text{V}_3$ ) barrier for the methyl internal rotation was determined to be  $1173.7 \text{ cm}^{-1}$  (Pearson et al. 1995) and  $1331 \text{ cm}^{-1}$  (Kakar & Quade 1980) in the trans and gauche substates of the ground vibrational state, respectively. Since these barriers are rather high, transitions of the ground state A and E components occur with less than 1 MHz separation. The A/E splittings can often be resolved in the trans substate, but can rarely be resolved in the gauche substates. In the submillimeter region, methyl torsional splittings are almost never resolved and are effectively averaged by any measurements. Any resolved methyl torsional splittings have been averaged in this treatment of ethanol.

The potential for the motion of the OH proton has a global minimum (the trans well) that corresponds to the hydroxyl proton lying in the CCO plane. Two secondary minima (the gauche wells) occur when the proton lies approximately  $120^\circ$  from the trans minimum (Pearson et al. 1996). Figure 1 shows the potential based on some recent work of Su & Quade (1996). The energy difference between the trans and gauche minima is due to the departure from perfect threefold symmetry. The plane of symmetry containing the trans minimum can be used to describe the symmetry of torsional wave functions with the  $\text{C}_s$  symmetry group. Solution of the torsional wave equation results in a series of wave functions which are symmetric (e) or anti-symmetric (o) about the CCO plane of symmetry and can be labeled by the number of nodes. Since the barrier is predominantly threefold, each torsional state is divided into three substates. The lowest energy wave function,  $e_0$ , or trans, has no nodes, is symmetric, and peaks in amplitude at

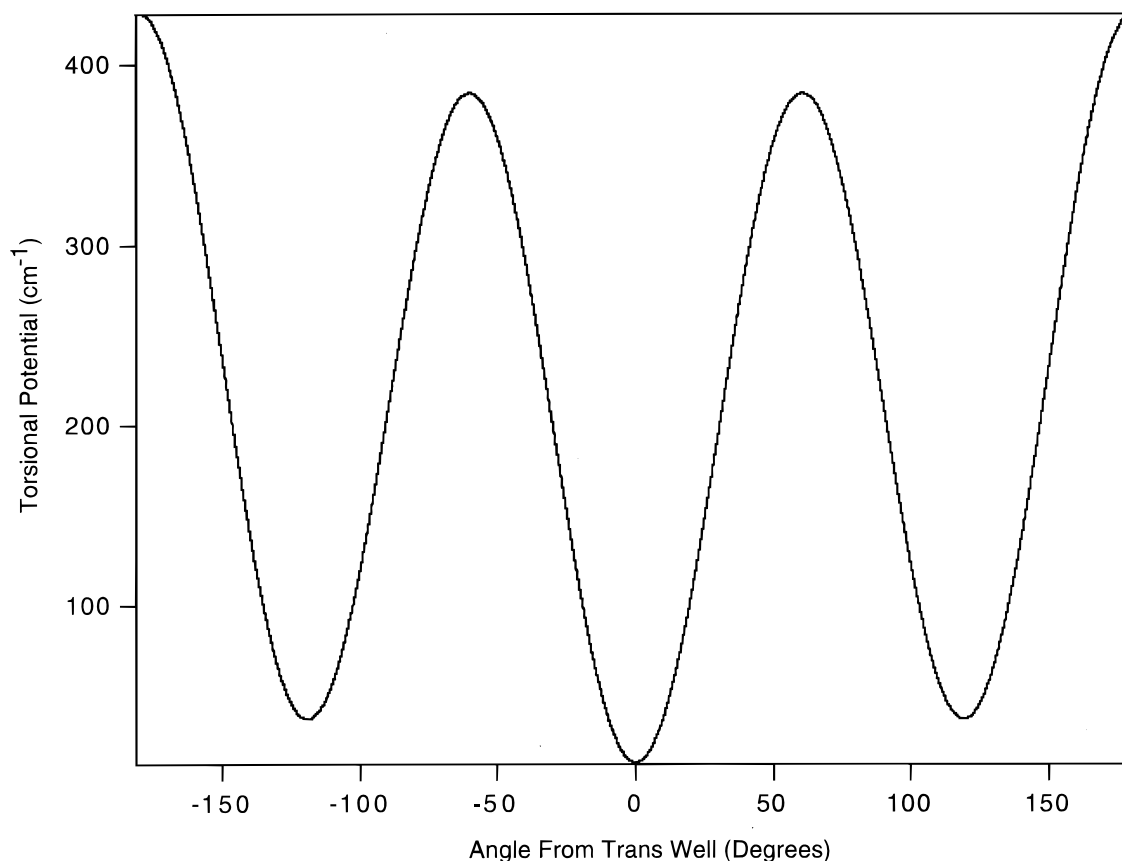


FIG. 1.—Potential energy for torsional motion of the hydroxyl proton in ethanol shown as a function of torsional angle, measured from the trans configuration, at which the potential is a minimum. The two different gauche wells are equivalent and lie slightly higher in energy than the trans well.

the trans minimum. The next two wave functions have one node each and comprise a closely spaced symmetric ( $e_1$  or gauche+) and antisymmetric ( $o_1$  or gauche-) pair with amplitude peaks at the gauche potential minima. Ground state torsional wave functions computed with the potential of Su & Quade (1996) are shown in Figure 2. These wave functions are significantly less localized than those calculated from the previous potential of Kakar & Quade (1980), which contains a slightly higher barrier.

The selection rules determined by the  $C_s$  group allow  $a$ - and  $b$ -type transitions between substates of the same symmetry and  $c$ -type transitions between substates of different symmetries. As a result,  $a$ - and  $b$ -type transitions are formally allowed within each torsional substate and between trans and gauche+, while  $c$ -type transitions are allowed between gauche+ and gauche- and trans and gauche-.

The reported dipole moments for ethanol are given in matrix form in Table 1. In the trans substate, the  $b$ -component of the dipole moment dominates, while the  $a$ -component is quite small. In the gauche torsional substates, the  $a$ -component of the dipole is large and the  $b$ -component small. It should be noted that no trans  $a$ -type or gauche  $b$ -type transitions have been observed in the absence of large level mixing. The line strengths predicted from the dipole moment components reported for these states should lead to observation of transitions; however, these transitions have not been detected in spectrometer systems with high sensitivity, suggesting that the effective transition moments may be significantly smaller than previously reported. It should also be noted that the dipole components were determined using analyses that excluded many important interactions among the substates of the

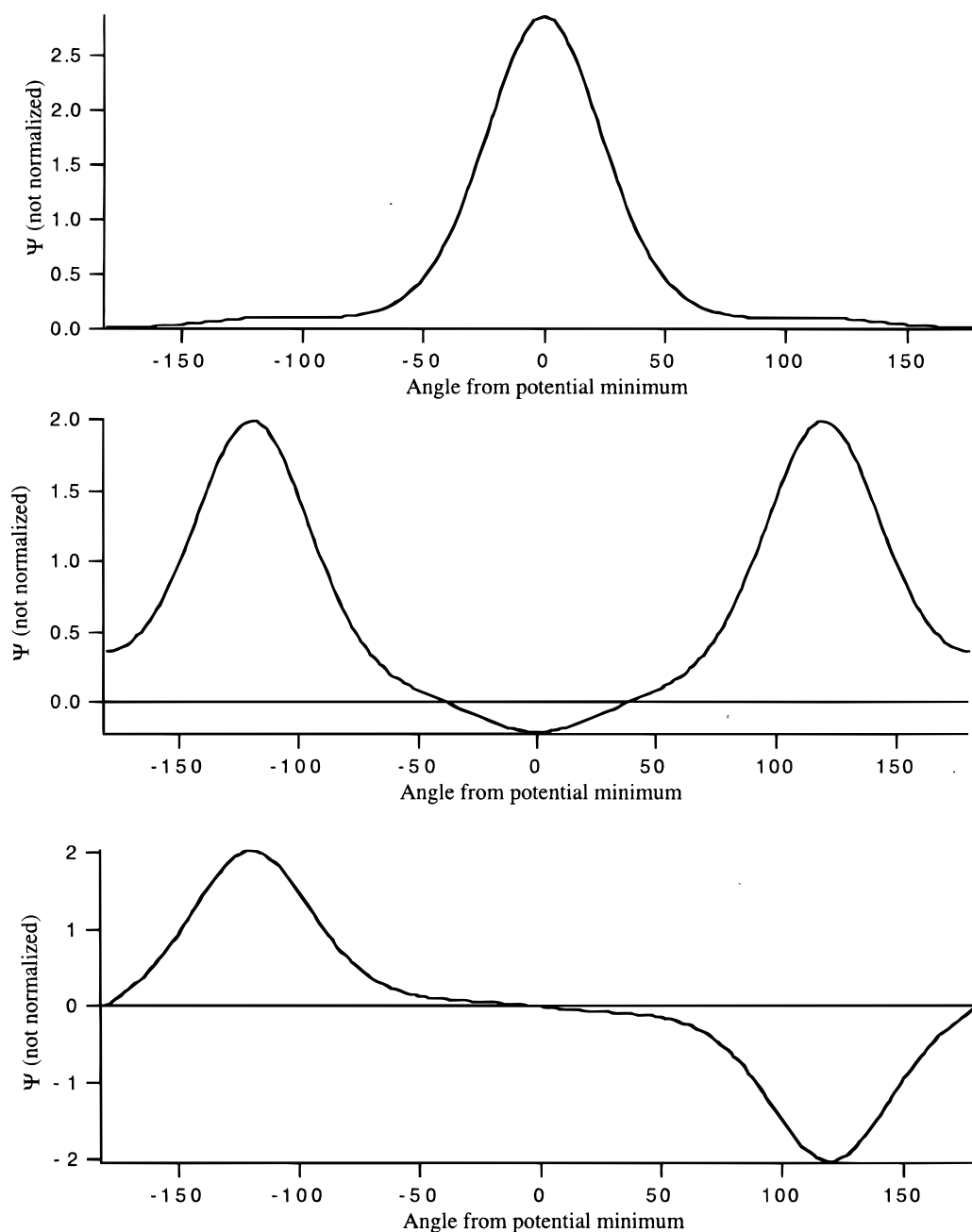


FIG. 2.—Calculated unnormalized wave functions for the lowest lying trans (top), gauche+ (middle), and gauche- (bottom) torsional substates

TABLE 1  
TRANSITION DIPOLE MATRIX

|                | Trans                                                                         | Gauche +                                                                      | Gauche -                                                                      |
|----------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
| Trans .....    | $\mu_a = 0.046 \text{ D}^a$<br>$\mu_b = 1.438 \text{ D}^a$<br>$\mu_c = 0.0^b$ | $\mu_a = \text{NA}$<br>$\mu_b = \text{NA}$<br>$\mu_c = 0.0^b$                 | $\mu_a = 0.0^b$<br>$\mu_b = 0.0^b$<br>$\mu_c = \text{NA}$                     |
| Gauche + ..... | $\mu_a = \text{NA}$<br>$\mu_b = \text{NA}$<br>$\mu_c = 0.0^b$                 | $\mu_a = 1.264 \text{ D}^c$<br>$\mu_b = 0.104 \text{ D}^c$<br>$\mu_c = 0.0^b$ | $\mu_a = 0.0^b$<br>$\mu_b = 0.0^b$<br>$\mu_c = 1.101 \text{ D}^c$             |
| Gauche - ..... | $\mu_a = 0.0^b$<br>$\mu_b = 0.0^b$<br>$\mu_c = \text{NA}$                     | $\mu_a = 0.0^b$<br>$\mu_b = 0.0^b$<br>$\mu_c = 1.101 \text{ D}^c$             | $\mu_a = 1.264 \text{ D}^c$<br>$\mu_b = 0.104 \text{ D}^c$<br>$\mu_c = 0.0^b$ |

NOTES.—The symbol NA means not available. Transition dipoles listed as NA are probably small and are fixed to zero in the calculations reported here. The symbol D stands for Debye ( $1 \text{ D} = 10^{-18} \text{ esu cm}$ ).

<sup>a</sup> Takano, Sasada, & Satoh 1968.

<sup>b</sup> From symmetry.

<sup>c</sup> Kakar & Quade 1980.

ground vibrational state. Symmetry-allowed transition moments between the trans and gauche substates are not known and are listed as “not available” in Table 1. The trans to gauche transition moments are expected to be small due to limited torsional overlap between these substates.

We have previously discussed a suitable Hamiltonian for OH torsional motion in ethanol and its interaction with the overall rotational motion (Pearson et al. 1996). The Hamiltonian  $H$ , derived and applied by Quade and coworkers (Quade & Lin 1963; Quade 1966, 1967; Knopp & Quade 1968), can be divided into three terms:

$$H = H_R + H_{\text{TR}} + H_T. \quad (1)$$

Here  $H_R$  is the rigid-body rotational Hamiltonian with centrifugal distortion,  $H_T$  is the torsional Hamiltonian, and  $H_{\text{TR}}$  is the torsion-rotation interaction. A variety of steps lead to an effective Hamiltonian which contains operators similar to those used in treating Coriolis and Fermi interactions between vibrational states. This effective Hamiltonian  $H$  is given to second order in angular momentum by the expressions

$$\begin{aligned} H_R &= A^{(\sigma)} P_a^2 + B^{(\sigma)} P_b^2 + C^{(\sigma)} P_c^2 + F^{(\sigma)} (P_a P_b + P_b P_a) \\ H_{\text{TR}} &= D^{(\sigma^1, \sigma^2)} (P_b P_c + P_c P_b) + E^{(\sigma^1, \sigma^2)} (P_c P_a + P_a P_c) \\ &\quad + F^{(\sigma^1, \sigma^2)} (P_a P_b + P_b P_a) + M^{(\sigma^1, \sigma^2)} P_c + N^{(\sigma^1, \sigma^2)} P_b \\ &\quad + Q^{(\sigma^1, \sigma^2)} P_a + R^{(\sigma^1, \sigma^2)} (P_b^2 - P_c^2) + S^{(\sigma^1, \sigma^2)} P_a^2 \\ H_T &= \Delta E^{(\sigma)}, \end{aligned} \quad (2)$$

where the  $P_i$  are the components of angular momentum along the principal axes ( $i = a, b, c$ ) and the spectroscopic constants contain superscripts  $\sigma$  which refer to torsional substate. The procedure is referred to as the fixed-framework axis method (FFAM). In the FFAM formulation, all the  $H_{\text{TR}}$  terms connect two different torsional substates, so that the spectroscopic constants have two superscripts  $\sigma^1 \neq \sigma^2$ . An  $H_R$  term exists for each substate; setting  $F^{(\sigma)}$  to zero for one of the substates defines the axis system of the entire molecule as the effective principal axes of that substate (trans in this case). The  $H_T$  terms do not contain kinetic and potential energy expressions relating to torsional motion; rather, they are simply parameters which define the energies of the gauche substates with respect to the trans substate. In addition to expanding the  $H_R$  terms to

include higher order angular momentum terms, all the operators off diagonal in torsional substate can be expanded (Pearson et al. 1996) in order to help account for the higher order effects of the torsion and torsion-rotation interactions that are only approximately treated in this Hamiltonian formulation.

The  $C_s$  symmetry group dictates which of the  $H_{\text{TR}}$  terms possess nonzero off-diagonal matrix elements and which set of substates are linked by those elements, as discussed in our earlier work (Pearson et al. 1996). Here we briefly discuss the inclusion of these terms for trans-gauche interactions. Their effect is to produce perturbations from normal asymmetric top energy level patterns, selection rules, and intensities. In addition to possessing a dependence on torsional substate, the off-diagonal matrix elements also depend on the angular momentum quantum numbers. Since the total angular momentum  $J$  is a good quantum number,  $H_{\text{TR}}$  connects only those pairs of rotational levels in different torsional substates with the same total angular momentum  $J$ . To understand the dependence of nonzero matrix elements on the “pseudo” quantum numbers  $K_a$  and  $K_c$ , let us first consider ethanol to be a prolate symmetric top so that  $K_a$  is a real quantum number. In this limit, nonzero off-diagonal elements for the trans-gauche interactions exist for  $\Delta K_a = 0, \pm 1, \pm 2$ . The true asymmetric top functions, however, contain many different  $K_a$  quantum numbers (the designated quantum numbers  $K_a$  and  $K_c$  only refer to the most important prolate and oblate basis functions) so that trans-gauche interactions can occur when  $K_a$  changes by any amount. For interactions between the trans and the gauche + substates,  $K_c$  must change by an even amount ( $\Delta K_c = 0, \pm 2$  in the oblate symmetric top limit) and for interactions between the trans and gauche - substates,  $K_c$  must change by an odd amount ( $\Delta K_c = \pm 1$  in the oblate symmetric top limit). Unfortunately, these rules do not hold in all instances, since the gauche substates are often mixed (Pearson et al. 1996). Despite this great complexity, the analysis of interactions is aided by the general fact that the strongest interactions between pairs of rotational levels involve the smallest changes in  $K_a$  and the most closely spaced energy levels computed without interactions (this assertion is quantified in the next section). In particular, when two series of energy levels, each denoted by  $K_a$  and  $K_c$ , are plotted against  $J$ , it can be seen that interactions are strongest at so-called “level crossings.” In our earlier work on the spectra of the gauche torsional substates, we included only interactions between those two substates. In this paper, we have utilized a full three-substate formulation, which is the first time, to the best of our knowledge, that three states, including two of the same symmetry (trans and gauche +), have been analyzed with the FFAM method. Although our more complex analysis does not yet allow us to analyze all of the measured transitions, it has facilitated a considerable extension in the  $J$  and  $K_a$  range of our earlier work.

### 3. ANALYSIS

During the course of our investigations on the millimeter-wave and submillimeter-wave spectrum of ethanol (Pearson et al. 1995, 1996; this work), laboratory measurements were undertaken using five different spectrometer systems. The details of these spectrometer systems can be found elsewhere (Helminger, Messer, & De Lucia 1983; Booker, Crownover, & De Lucia 1988; King & Gordy 1953; Friedl

et al. 1995). A number of additional 12–26 GHz transitions have been assigned from a survey reported by Michielsen-Effinger (1962).

Our ground vibrational state data set now contains approximately 3500 measured transitions with typical uncertainties of 50 kHz, of which approximately 1600 have appeared previously in the literature (Pearson et al. 1995, 1996). The analyzed transitions lie between 8 and 652 GHz and cover a  $J$  and  $K_a$  range of 50 and 17, respectively. The present three-state model fits all 3500 transitions with a root mean square deviation of 400 kHz, with the majority fitting to near experimental accuracy (50–100 kHz). Despite a few remaining problems, the current analysis successfully fit many transitions shifted more than 1 GHz by previously neglected trans-gauche interactions. Although our spectroscopic work is incomplete, we are currently able to report a variety of astronomically interesting and perturbed gauche— to gauche+ spectral branches. These branches were partially analyzed in our previous work, but now we have been able to analyze these branches to a much higher  $J$  quantum number. A complete list of spectral transitions along with a comprehensive analysis will appear later.

We have divided the newly analyzed spectral lines into two tables. Table 2 contains gauche—–gauche+  $K_a = 0, 1$  and  $K_c = J$   $^cQ$ -branches ( $\Delta J = 0$ ,  $\Delta K_a = \pm 1$ ,  $\Delta K_c = 0$ ) along with perturbation allowed  $^xQ$  transitions ( $\Delta J = 0$ ,  $\Delta K_a = 0$ ,  $\Delta K_c = 0$ ) between the same levels where seen.

Table 3 contains gauche—–gauche+  $K_a = 1, 2$  and  $K_c = J - 1$   $^cQ$ -branches along with perturbation-allowed  $^xQ$  transitions between the same levels where seen. Some of the lower  $J$  lines ( $J < 30$ ) in the tables were also analyzed with our previous two-state analysis (Pearson et al. 1996). These two tables include the quantum numbers, the measured frequencies, the observed minus the calculated frequencies, the intensities in terms of  $\mu_x^2 {}^xS_{ba}$ , (the dipole component squared multiplied by the line strength), the lower state energies, and selected notes. The intensities are based on the transition moments in Table 1, with all unknown values assumed to be zero. In Tables 2 and 3, the gauche+ state is denoted by  $t = 0$  and the gauche— state by  $t = 1$ . A significant number of the transitions involve highly perturbed levels and are denoted in the note column with “gg” for a gauche+ gauche— perturbation or “tg” for a trans-gauche perturbation. Note that although the designated tg perturbations have their onset at high  $J$ , such interactions are important at lower  $J$  as well.

To provide a feel for the trans-gauche (tg) interactions involved in the three-state analysis, we have shown trans-gauche level crossings for gauche  $J(0, J)$  and  $J(1, J)$  levels in Figure 3, and trans-gauche level crossings for gauche  $J(1, J - 1)$  and  $J(2, J - 1)$  levels in Figure 4. The gauche levels in Figure 3 are the energy levels which are connected by the transitions in Table 2 while the gauche levels in Figure 4 are the levels connected by the transitions listed in

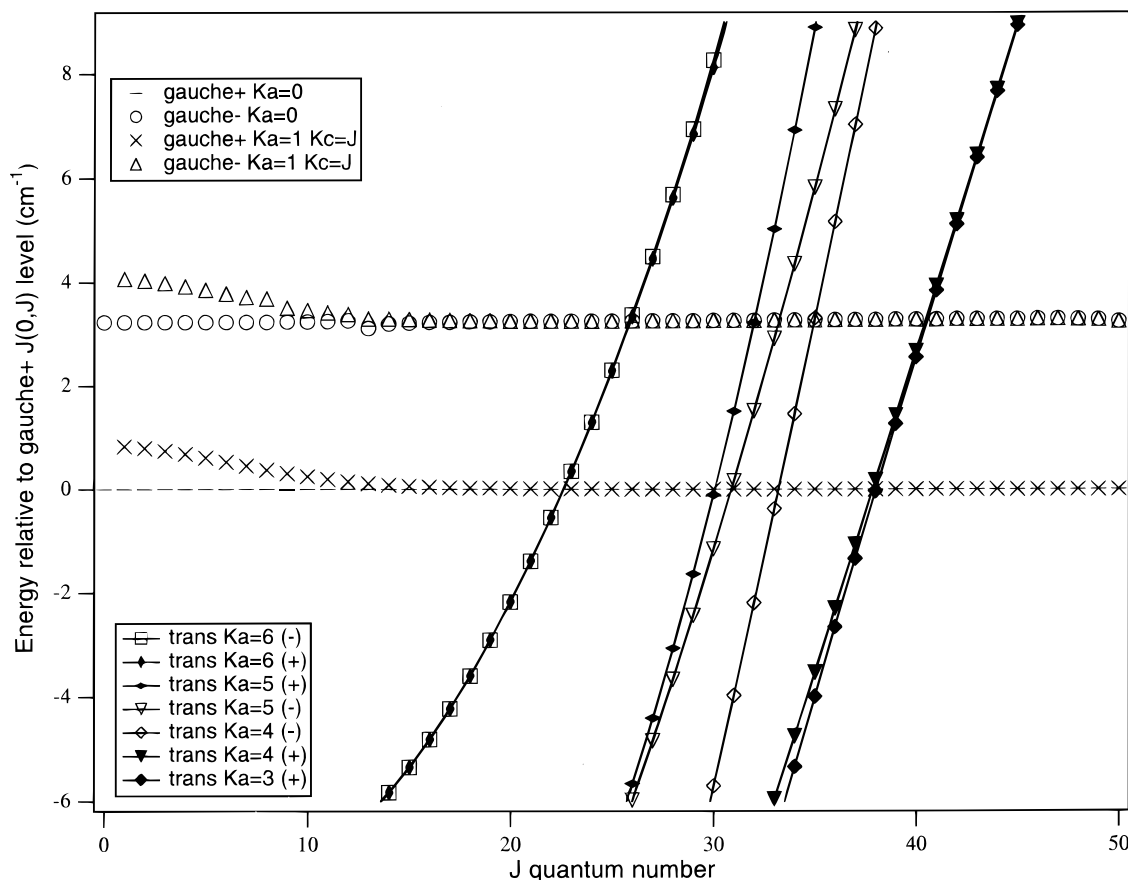


FIG. 3.—Crossings between two selected gauche+ and two selected gauche— rotational-torsional levels involved in the transitions analyzed here [ $J(0, J)$ ,  $J(1, J)$ ] with assorted rotational levels of the trans substate. Energies relative to the lowest gauche rotational torsional level [gauche+;  $J(0, J)$ ] are plotted vs. total angular momentum quantum number  $J$ . At the crossings, perturbations which necessitate our current three-state analysis are at their maximum values. For a given series of rotational levels in the trans substate, interactions occur either with the gauche+ or gauche— levels; these possibilities are indicated by + and —, respectively, in the labeling of the trans substate series.

TABLE 2  
GAUCHE – GAUCHE +  ${}^cQ$  AND  ${}^sQ$  BRANCHES WITH  $K_a = 0$  OR 1 AND  $K_c = J$

| $J'$ | $K'_a$ | $K'_c$ | $t'$ | $J''$ | $K''_a$ | $K''_c$ | $t''$ | Frequency<br>(MHz) | $O - C$ | $\mu^2 S^a$ | $E_{\text{lower}}$<br>( $\text{cm}^{-1}$ ) | Notes |
|------|--------|--------|------|-------|---------|---------|-------|--------------------|---------|-------------|--------------------------------------------|-------|
| 1    | 0      | 1      | 1    | 1     | 1       | 1       | 0     | 71918.992          | −0.420  | 1.8         | 40.9458                                    |       |
| 1    | 1      | 1      | 1    | 1     | 0       | 1       | 0     | 121933.986         | −0.288  | 1.8         | 40.1173                                    |       |
| 2    | 0      | 2      | 1    | 2     | 1       | 2       | 0     | 72986.578          | −0.470  | 3.1         | 42.0628                                    |       |
| 2    | 1      | 2      | 1    | 2     | 0       | 2       | 0     | 120900.880         | −0.279  | 3.0         | 41.2695                                    |       |
| 3    | 0      | 3      | 1    | 3     | 1       | 3       | 0     | 74519.642          | −0.400  | 4.4         | 43.7376                                    |       |
| 3    | 1      | 3      | 1    | 3     | 0       | 3       | 0     | 119420.966         | −0.289  | 4.5         | 42.9949                                    |       |
| 4    | 0      | 4      | 1    | 4     | 1       | 4       | 0     | 76437.327          | −0.378  | 6.1         | 45.9694                                    |       |
| 4    | 1      | 4      | 1    | 4     | 0       | 4       | 0     | 117579.752         | −0.247  | 5.9         | 45.2899                                    |       |
| 5    | 0      | 5      | 1    | 5     | 1       | 5       | 0     | 78637.457          | −0.334  | 7.6         | 48.7569                                    |       |
| 5    | 1      | 5      | 1    | 5     | 0       | 5       | 0     | 115494.515         | −0.220  | 7.4         | 48.1501                                    |       |
| 6    | 0      | 6      | 1    | 6     | 1       | 6       | 0     | 81003.969          | −0.287  | 9.5         | 52.0990                                    |       |
| 6    | 1      | 6      | 1    | 6     | 0       | 6       | 0     | 113325.517         | −0.157  | 9.1         | 51.5703                                    |       |
| 7    | 0      | 7      | 1    | 7     | 1       | 7       | 0     | 83417.055          | −0.237  | 11.4        | 55.9943                                    |       |
| 7    | 1      | 7      | 1    | 7     | 0       | 7       | 0     | 111344.327         | −0.104  | 9.4         | 55.5448                                    |       |
| 8    | 0      | 8      | 1    | 8     | 1       | 8       | 0     | 85765.145          | −0.172  | 13.7        | 60.4413                                    |       |
| 8    | 1      | 8      | 1    | 8     | 0       | 8       | 0     | 110368.495         | −0.051  | 8.1         | 60.0682                                    |       |
| 9    | 0      | 9      | 1    | 9     | 1       | 9       | 0     | 87959.044          | −0.053  | 15.6        | 65.4384                                    |       |
| 9    | 0      | 9      | 1    | 9     | 0       | 9       | 0     | 97034.628          | −0.007  | 0.1         | 65.1357                                    |       |
| 9    | 1      | 9      | 1    | 9     | 0       | 9       | 0     | 105162.089         | −0.172  | 14.7        | 65.1357                                    |       |
| 10   | 0      | 10     | 1    | 10    | 1       | 10      | 0     | 89946.985          | −0.061  | 18.2        | 70.9843                                    |       |
| 10   | 0      | 10     | 1    | 10    | 0       | 10      | 0     | 97159.134          | 0.052   | 0.1         | 70.7437                                    |       |
| 10   | 1      | 10     | 1    | 10    | 1       | 10      | 0     | 96584.856          | −0.160  | 0.2         | 70.9843                                    |       |
| 10   | 1      | 10     | 1    | 10    | 0       | 10      | 0     | 103796.950         | −0.101  | 16.5        | 70.7437                                    |       |
| 11   | 0      | 11     | 1    | 11    | 1       | 11      | 0     | 91737.109          | 0.067   | 19.4        | 77.0774                                    | gg    |
| 11   | 0      | 11     | 1    | 11    | 0       | 11      | 0     | 97363.587          | 0.170   | 0.4         | 76.8897                                    | gg    |
| 11   | 1      | 11     | 1    | 11    | 1       | 11      | 0     | 96862.936          | −0.137  | 0.1         | 77.0774                                    | gg    |
| 11   | 1      | 11     | 1    | 11    | 0       | 11      | 0     | 102489.386         | −0.065  | 20.3        | 76.8897                                    | gg    |
| 12   | 0      | 12     | 1    | 12    | 1       | 12      | 0     | 93477.574          | 0.280   | 21.1        | 83.7165                                    | gg    |
| 12   | 0      | 12     | 1    | 12    | 0       | 12      | 0     | 97797.282          | 0.394   | 1.3         | 83.5724                                    | gg    |
| 12   | 1      | 12     | 1    | 12    | 1       | 12      | 0     | 97214.225          | −0.104  | 1.1         | 83.7165                                    | gg    |
| 12   | 1      | 12     | 1    | 12    | 0       | 12      | 0     | 101533.895         | −0.028  | 20.6        | 83.5724                                    | gg    |
| 13   | 0      | 13     | 1    | 13    | 1       | 13      | 0     | 90007.707          | −1.210  | 15.7        | 90.9003                                    | gg    |
| 13   | 0      | 13     | 1    | 13    | 0       | 13      | 0     | 93279.005          | −1.122  | 2.1         | 90.7912                                    | gg    |
| 13   | 1      | 13     | 1    | 13    | 1       | 13      | 0     | 95607.001          | 0.423   | 7.6         | 90.9003                                    | gg    |
| 13   | 1      | 13     | 1    | 13    | 0       | 13      | 0     | 98878.281          | 0.494   | 15.7        | 90.7912                                    | gg    |
| 14   | 0      | 14     | 1    | 14    | 1       | 14      | 0     | 93497.421          | −0.780  | 24.4        | 98.6280                                    | gg    |
| 14   | 0      | 14     | 1    | 14    | 0       | 14      | 0     | 95946.145          | −0.700  | 0.5         | 98.5463                                    | gg    |
| 14   | 1      | 14     | 1    | 14    | 1       | 14      | 0     | 96534.856          | 0.072   | 0.9         | 98.6280                                    | gg    |
| 14   | 1      | 14     | 1    | 14    | 0       | 14      | 0     | 98983.548          | 0.121   | 26.3        | 98.5463                                    | gg    |
| 15   | 0      | 15     | 1    | 15    | 1       | 15      | 0     | 94696.400          | −0.456  | 31.1        | 106.8985                                   |       |
| 15   | 1      | 15     | 1    | 15    | 0       | 15      | 0     | 98585.095          | 0.079   | 31.2        | 106.8379                                   |       |
| 16   | 0      | 16     | 1    | 16    | 1       | 16      | 0     | 95416.540          | −0.351  | 32.1        | 115.7111                                   |       |
| 16   | 1      | 16     | 1    | 16    | 0       | 16      | 0     | 98230.313          | 0.035   | 32.4        | 115.6666                                   |       |
| 17   | 0      | 17     | 1    | 17    | 1       | 17      | 0     | 95924.464          | −0.264  | 36.1        | 125.0652                                   |       |
| 17   | 1      | 17     | 1    | 17    | 0       | 17      | 0     | 97962.858          | 0.059   | 36.1        | 125.0327                                   |       |
| 18   | 0      | 18     | 1    | 18    | 1       | 18      | 0     | 96301.823          | −0.198  | 37.3        | 134.9602                                   |       |
| 18   | 1      | 18     | 1    | 18    | 0       | 18      | 0     | 97774.307          | 0.042   | 37.4        | 134.9367                                   |       |
| 19   | 0      | 19     | 1    | 19    | 1       | 19      | 0     | 96589.759          | −0.156  | 40.9        | 145.3958                                   |       |
| 19   | 1      | 19     | 1    | 19    | 0       | 19      | 0     | 97649.502          | 0.051   | 40.9        | 145.3788                                   |       |
| 20   | 0      | 20     | 1    | 20    | 1       | 20      | 0     | 96814.209          | −0.131  | 42.2        | 156.3715                                   |       |
| 20   | 1      | 20     | 1    | 20    | 0       | 20      | 0     | 97574.042          | 0.070   | 42.3        | 156.3593                                   |       |
| 21   | 0      | 21     | 1    | 21    | 1       | 21      | 0     | 96993.103          | −0.081  | 45.6        | 167.8871                                   |       |
| 21   | 1      | 21     | 1    | 21    | 0       | 21      | 0     | 97535.908          | 0.027   | 45.6        | 167.8784                                   |       |
| 22   | 0      | 22     | 1    | 22    | 1       | 22      | 0     | 97139.012          | −0.024  | 47.0        | 179.9424                                   |       |
| 22   | 1      | 22     | 1    | 22    | 0       | 22      | 0     | 97525.798          | 0.060   | 47.1        | 179.9362                                   |       |
| 23   | 0      | 23     | 1    | 23    | 1       | 23      | 0     | 97263.582          | −0.048  | 50.3        | 192.5370                                   |       |
| 23   | 1      | 23     | 1    | 23    | 0       | 23      | 0     | 97536.849          | 0.119   | 50.3        | 192.5326                                   |       |
| 24   | 0      | 24     | 1    | 24    | 1       | 24      | 0     | 97369.131          | −0.014  | 51.8        | 205.6709                                   |       |
| 24   | 1      | 24     | 1    | 24    | 0       | 24      | 0     | 97562.844          | 0.100   | 51.8        | 205.6678                                   |       |
| 25   | 0      | 25     | 1    | 25    | 1       | 25      | 0     | 97463.716          | 0.023   | 55.0        | 219.3439                                   |       |
| 25   | 1      | 25     | 1    | 25    | 0       | 25      | 0     | 97600.390          | 0.085   | 55.0        | 219.3417                                   |       |
| 26   | 0      | 26     | 1    | 26    | 1       | 26      | 0     | 97549.692          | 0.011   | 56.5        | 233.5558                                   |       |
| 26   | 1      | 26     | 1    | 26    | 0       | 26      | 0     | 97645.192          | 0.019   | 56.5        | 233.5542                                   |       |
| 27   | 0      | 27     | 1    | 27    | 1       | 27      | 0     | 97631.329          | 0.160   | 59.6        | 248.3065                                   |       |
| 27   | 1      | 27     | 1    | 27    | 0       | 27      | 0     | 97698.530          | 0.056   | 59.6        | 248.3054                                   |       |
| 28   | 0      | 28     | 1    | 28    | 1       | 28      | 0     | 97708.888          | 0.114   | 61.2        | 263.5958                                   |       |
| 28   | 1      | 28     | 1    | 28    | 0       | 28      | 0     | 97755.610          | 0.063   | 61.2        | 263.5950                                   |       |
| 29   | 0      | 29     | 1    | 29    | 1       | 29      | 0     | 97784.113          | 0.133   | 64.1        | 279.4236                                   |       |
| 29   | 1      | 29     | 1    | 29    | 0       | 29      | 0     | 97815.987          | 0.051   | 64.1        | 279.4231                                   |       |
| 30   | 0      | 30     | 1    | 30    | 1       | 30      | 0     | 97857.476          | 0.152   | 63.4        | 295.7898                                   | tg    |
| 30   | 0      | 30     | 1    | 30    | 0       | 30      | 0     | 97865.529          | 0.165   | 2.4         | 295.7896                                   | tg    |
| 30   | 1      | 30     | 1    | 30    | 1       | 30      | 0     | 97869.443          | 0.169   | 2.4         | 295.7898                                   | tg    |

TABLE 2—Continued

| $J'$ | $K'_a$ | $K'_c$ | $t'$ | $J''$ | $K''_a$ | $K''_c$ | $t''$ | Frequency<br>(MHz)     | $O-C$  | $\mu^2 S^a$ | $E_{\text{lower}}$<br>( $\text{cm}^{-1}$ ) | Notes |
|------|--------|--------|------|-------|---------|---------|-------|------------------------|--------|-------------|--------------------------------------------|-------|
| 30   | 1      | 30     | 1    | 30    | 0       | 30      | 0     | 97877.456              | 0.056  | 63.4        | 295.7896                                   | tg    |
| 31   | 1      | 31     | 1    | 31    | 0       | 31      | 0     | 97998.068              | 0.021  | 63.3        | 312.6923                                   | tg    |
| 31   | 1      | 31     | 1    | 31    | 1       | 31      | 0     | 97940.731              | 0.019  | 4.9         | 312.6943                                   | tg    |
| 31   | 0      | 31     | 1    | 31    | 0       | 31      | 0     | 97989.809              | 0.198  | 4.9         | 312.6923                                   | tg    |
| 31   | 0      | 31     | 1    | 31    | 1       | 31      | 0     | 97932.445              | -0.004 | 63.9        | 312.6943                                   | tg    |
| 32   | 1      | 32     | 1    | 32    | 0       | 32      | 0     | 98021.302              | 0.146  | 20.2        | 330.1364                                   | tg    |
| 32   | 0      | 32     | 1    | 32    | 0       | 32      | 0     | 98039.493              | -0.031 | 49.7        | 330.1364                                   | tg    |
| 32   | 1      | 32     | 1    | 32    | 1       | 32      | 0     | 98006.956              | -0.040 | 50.3        | 330.1369                                   | tg    |
| 32   | 0      | 32     | 1    | 32    | 1       | 32      | 0     | 98025.137              | 0.022  | 19.8        | 330.1369                                   | tg    |
| 33   | 1      | 33     | 1    | 33    | 0       | 33      | 0     | 98091.912              | 0.003  | 64.5        | 348.1170                                   | tg    |
| 33   | 0      | 33     | 1    | 33    | 0       | 33      | 0     | 98087.678              | 0.034  | 8.8         | 348.1170                                   | tg    |
| 33   | 1      | 33     | 1    | 33    | 1       | 33      | 0     | 98060.630 <sup>b</sup> | 0.055  | 8.8         | 348.1181                                   | tg, B |
| 33   | 0      | 33     | 1    | 33    | 1       | 33      | 0     | 98056.249              | 0.168  | 64.4        | 348.1181                                   | tg    |
| 34   | 1      | 34     | 1    | 34    | 1       | 34      | 0     | 98163.428 <sup>b</sup> | 0.042  | 48.0        | 366.6354                                   | tg, B |
| 34   | 0      | 34     | 1    | 34    | 0       | 34      | 0     | 98163.428 <sup>b</sup> | 0.128  | 48.0        | 366.6353                                   | tg, B |
| 34   | 0      | 34     | 1    | 34    | 1       | 34      | 0     | 98160.391              | -0.042 | 27.0        | 366.6354                                   | tg    |
| 34   | 1      | 34     | 1    | 34    | 0       | 34      | 0     | 98166.466              | 0.013  | 27.0        | 366.6353                                   | tg    |
| 35   | 1      | 35     | 1    | 35    | 0       | 35      | 0     | 98237.509              | 0.075  | 64.2        | 385.6915                                   | tg    |
| 35   | 0      | 35     | 1    | 35    | 0       | 35      | 0     | 98235.479              | 0.021  | 13.7        | 385.6915                                   | tg    |
| 35   | 1      | 35     | 1    | 35    | 1       | 35      | 0     | 98236.443              | 0.025  | 13.7        | 385.6915                                   | tg    |
| 35   | 0      | 35     | 1    | 35    | 1       | 35      | 0     | 98234.400              | -0.004 | 64.2        | 385.6915                                   | tg    |
| 36   | 0      | 36     | 1    | 36    | 1       | 36      | 0     | 98309.847              | -0.012 | 76.6        | 405.2851                                   |       |
| 36   | 1      | 36     | 1    | 36    | 0       | 36      | 0     | 98312.053              | -0.028 | 76.6        | 405.2851                                   |       |
| 37   | 0      | 37     | 1    | 37    | 1       | 37      | 0     | 98386.495              | -0.114 | 81.6        | 425.4160                                   |       |
| 37   | 1      | 37     | 1    | 37    | 0       | 37      | 0     | 98388.088              | -0.105 | 81.6        | 425.4160                                   |       |
| 38   | 0      | 38     | 1    | 38    | 1       | 38      | 0     | 98464.381              | -0.175 | 84.1        | 446.0842                                   |       |
| 38   | 1      | 38     | 1    | 38    | 0       | 38      | 0     | 98465.570              | -0.177 | 84.1        | 446.0842                                   | tg    |
| 39   | 0      | 39     | 1    | 39    | 1       | 39      | 0     | 98544.249              | -0.262 | 83.0        | 467.2895                                   | tg    |
| 39   | 1      | 39     | 1    | 39    | 0       | 39      | 0     | 98545.375              | -0.297 | 83.0        | 467.289                                    |       |
| 40   | 0      | 40     | 1    | 40    | 1       | 40      | 0     | 98634.200              | -0.583 | 74.1        | 489.0317                                   | tg    |
| 40   | 1      | 40     | 1    | 40    | 0       | 40      | 0     | 98638.544              | -0.750 | 74.1        | 489.0317                                   | tg    |

NOTES.—(B) Blend; (gg) gauche + -gauche - interaction; (tg) trans-gauche interaction. See also Fig. 3.

<sup>a</sup> Units are Debye squared.

<sup>b</sup> Uncertainty of 250 kHz.

Table 3. The gauche levels, plotted as a function of  $J$  with respect to the lowest level of the four depicted, are shown as the horizontal or nearly horizontal lines. Gauche-gauche (gg) interactions, which peak at  $J = 13$  and  $J = 18$ , are especially noticeable in Figure 4. To illustrate possible interactions with trans levels, the energies of selected trans levels defined by  $K_a$  are also shown. These energies increase more rapidly as functions of  $J$  and cross the gauche levels; at the crossings, interactions are noticeable even if the  $K_a$  values of the gauche and trans levels differ by wide amounts. The (+) and (-) shown after the labeling of the trans levels refer to the symmetry of the interacting gauche substate. The strength of the interaction between levels that cross in the absence of torsional rotational interaction decreases about 1 order of magnitude for each quantum of  $K_a$  difference, with the  $\Delta K_a = 2$  interactions being about 3 GHz and  $\Delta K_a = 5$  interactions being about 3 MHz.

#### 4. ASTRONOMICAL ASSIGNMENTS

The  $U$  lines from Ohishi et al. (1988) that are believed to be caused by ethanol are given in Table 4. The observed  $U$  line frequencies, measured (laboratory) rest frequencies,  $T_A^*$ ,  $\Delta v$ ,  $\mu^2 S$ , upper state energies, quantum assignments, and estimated  $v_{\text{LSR}}$  values are also given. The method used here for determining the total column density  $N$ , discussed by Blake et al. (1986) and Turner (1991), contains the assumption that the emission source is optically thin and characterized by a single excitation temperature  $T_{\text{rot}}$ . In this approximation, the logarithm of the upper state column

density  $N_u$  divided by the upper stage degeneracy  $g_u$  can be plotted against the upper state energy  $E_u/k$  in the following manner:

$$\log_{10} \left( \frac{N_u}{g_u} \right) = \log_{10} \left( \frac{3kW}{8\pi^3 v_{\text{ba}}^2 S_{\text{ba}} \mu_x^2} \right) = \log_{10} \left[ \frac{N}{Q_{\text{rs}}} \right] - \frac{E_u}{k} \left( \frac{\log_{10}(e)}{T_{\text{rot}}} \right), \quad (3)$$

so that the slope  $-\log_{10}(e)/T_{\text{rot}}$  and intercept  $\log_{10}(N/Q_{\text{rs}})$  contain the excitation temperature  $T_{\text{rot}}$  and the total column density  $N$  divided by the partition function  $Q_{\text{rs}}$ , respectively. Here  $W$  is the integrated line intensity which, with an assumed beam efficiency of 100%, is estimated to be  $T_A^*$  times the velocity linewidth  $\Delta v$ , and  $v_{\text{ba}}$  is the transition frequency.

In order to obtain an accurate partition function, the trans to gauche + tunneling frequency, or energy difference, must be known. This parameter is determined by the location of perturbations between trans and gauche levels and by the frequencies of several perturbation-allowed trans to gauche transitions. The best value for the energy difference between the rotationless trans and gauche + substates is  $1185399.1 \pm 5.0$  MHz, or  $39.54066 \pm 17 \times 10^{-4} \text{ cm}^{-1}$ . Although this number does not represent a final value, since our analysis is as yet incomplete, it is certainly sufficiently accurate to calculate column densities and rotational temperatures. Table 5 contains  $Q_{\text{rs}}$  values for a variety of temperatures, calculated with an explicit sum over all states of

TABLE 3  
GAUCHE+--GAUCHE--<sup>c</sup>Q- AND <sup>s</sup>Q BRANCHES WITH  $K_a = 1$  OR 2 AND  $K_c = J - 1$

| $J'$ | $K'_a$ | $K'_c$ | $t'$ | $J''$ | $K''_a$ | $K''_c$ | $t''$ | Frequency<br>(MHz)      | $O - C$ | $\mu^2 S^a$ | $E_{\text{lower}}^{\text{b}}$<br>(cm <sup>-1</sup> ) | Notes/<br>References |
|------|--------|--------|------|-------|---------|---------|-------|-------------------------|---------|-------------|------------------------------------------------------|----------------------|
| 2    | 1      | 1      | 1    | 2     | 2       | 1       | 0     | 22618.680               | -0.318  | 0.8         | 44.6573                                              | 1                    |
| 2    | 2      | 1      | 1    | 2     | 1       | 1       | 0     | 172641.532 <sup>b</sup> | -0.100  | 1.0         | 42.1717                                              | 2                    |
| 3    | 1      | 2      | 1    | 3     | 2       | 2       | 0     | 24288.620               | -0.301  | 2.1         | 46.3867                                              | 1                    |
| 3    | 2      | 2      | 1    | 3     | 1       | 2       | 0     | 171023.183 <sup>b</sup> | -0.491  | 1.7         | 43.9554                                              | 2                    |
| 4    | 1      | 3      | 1    | 4     | 2       | 3       | 0     | 26501.780               | -0.275  | 2.0         | 48.6916                                              | 1                    |
| 4    | 2      | 3      | 1    | 4     | 1       | 3       | 0     | 168882.814              | ...     | 2.5         | 46.3321                                              | P                    |
| 5    | 1      | 4      | 1    | 5     | 2       | 4       | 0     | 29255.850               | -0.187  | 3.8         | 51.5706                                              | 1                    |
| 5    | 2      | 4      | 1    | 5     | 1       | 4       | 0     | 166235.871              | 0.073   | 3.1         | 49.3005                                              |                      |
| 6    | 1      | 5      | 1    | 6     | 2       | 5       | 0     | 32570.910               | -0.136  | 3.1         | 55.0214                                              | 1                    |
| 6    | 2      | 5      | 1    | 6     | 1       | 5       | 0     | 163107.033              | ...     | 4.1         | 52.8589                                              | P                    |
| 7    | 1      | 6      | 1    | 7     | 2       | 6       | 0     | 36566.190               | -0.082  | 5.6         | 59.0378                                              | 1                    |
| 7    | 2      | 6      | 1    | 7     | 1       | 6       | 0     | 159531.132              | ...     | 4.7         | 57.0048                                              | P                    |
| 8    | 1      | 7      | 1    | 8     | 2       | 7       | 0     | 41903.357               | -0.011  | 1.8         | 63.5950                                              |                      |
| 8    | 2      | 7      | 1    | 8     | 1       | 7       | 0     | 155556.341              | ...     | 5.8         | 61.7354                                              | P                    |
| 9    | 1      | 8      | 1    | 9     | 2       | 8       | 0     | 43196.394               | -0.085  | 5.0         | 68.8693                                              |                      |
| 9    | 2      | 8      | 1    | 9     | 1       | 8       | 0     | 151249.647              | ...     | 6.6         | 67.0470                                              | P                    |
| 10   | 1      | 9      | 1    | 10    | 2       | 9       | 0     | 48378.176               | -0.090  | 7.9         | 74.5923                                              |                      |
| 10   | 2      | 9      | 1    | 10    | 1       | 9       | 0     | 146706.763              | ...     | 7.7         | 72.9347                                              | P                    |
| 11   | 1      | 10     | 1    | 11    | 2       | 10      | 0     | 53529.699               | -0.008  | 9.1         | 80.8901                                              |                      |
| 11   | 2      | 10     | 1    | 11    | 1       | 10      | 0     | 142083.013              | 0.617   | 8.8         | 79.3916                                              |                      |
| 12   | 1      | 11     | 1    | 12    | 2       | 11      | 0     | 58737.678               | 0.119   | 10.3        | 87.7546                                              |                      |
| 12   | 2      | 11     | 1    | 12    | 1       | 11      | 0     | 137749.076              | 0.927   | 8.5         | 86.4034                                              | gg                   |
| 13   | 1      | 12     | 1    | 13    | 2       | 12      | 0     | 63952.368               | -0.053  | 12.6        | 95.1823                                              |                      |
| 13   | 2      | 12     | 1    | 13    | 1       | 12      | 0     | 126566.577              | -0.034  | 5.3         | 94.2062                                              | gg                   |
| 14   | 1      | 13     | 1    | 14    | 2       | 13      | 0     | 69108.218               | -0.090  | 12.9        | 103.1705                                             |                      |
| 14   | 2      | 13     | 1    | 14    | 1       | 13      | 0     | 125279.125              | -0.044  | 15.9        | 102.2398                                             | gg                   |
| 15   | 1      | 14     | 1    | 15    | 2       | 14      | 0     | 74188.188               | -0.130  | 16.0        | 111.7166                                             |                      |
| 15   | 2      | 14     | 1    | 15    | 1       | 14      | 0     | 121496.294              | 0.211   | 15.4        | 110.9154                                             |                      |
| 16   | 1      | 15     | 1    | 15    | 2       | 15      | 0     | 79364.773               | ...     | 13.2        | 120.8184                                             | P                    |
| 16   | 2      | 15     | 1    | 16    | 1       | 15      | 0     | 117710.218              | 0.319   | 19.4        | 120.1491                                             |                      |
| 17   | 1      | 16     | 1    | 17    | 2       | 16      | 0     | 85419.515               | -0.153  | 14.0        | 130.4738                                             | gg                   |
| 17   | 2      | 16     | 1    | 17    | 1       | 16      | 0     | 114436.488              | 0.327   | 19.0        | 129.9256                                             |                      |
| 18   | 1      | 17     | 1    | 18    | 2       | 17      | 0     | 80605.135               | ...     | 22.7        | 140.6806                                             | P, gg                |
| 18   | 2      | 17     | 1    | 18    | 1       | 17      | 0     | 112894.167              | 0.038   | 13.1        | 140.2393                                             |                      |
| 19   | 1      | 18     | 1    | 19    | 2       | 18      | 0     | 84983.789               | -0.193  | 22.1        | 151.4369                                             | gg                   |
| 19   | 2      | 18     | 1    | 19    | 1       | 18      | 0     | 106931.232              | 0.436   | 23.5        | 151.0869                                             |                      |
| 20   | 1      | 19     | 1    | 20    | 2       | 19      | 0     | 88039.276               | -0.294  | 30.1        | 162.7410                                             |                      |
| 20   | 2      | 19     | 1    | 20    | 1       | 19      | 0     | 105225.485              | 0.424   | 30.4        | 162.460                                              |                      |
| 21   | 1      | 20     | 1    | 21    | 2       | 20      | 0     | 90354.336               | -0.404  | 29.2        | 174.5912                                             |                      |
| 21   | 2      | 20     | 1    | 21    | 1       | 20      | 0     | 103608.598              | 0.358   | 29.9        | 174.3793                                             |                      |
| 22   | 1      | 21     | 1    | 22    | 2       | 21      | 0     | 92156.495               | -0.428  | 34.9        | 186.9862                                             |                      |
| 22   | 2      | 21     | 1    | 22    | 1       | 21      | 0     | 102282.795              | 0.317   | 35.1        | 186.8239                                             |                      |
| 23   | 1      | 22     | 1    | 23    | 2       | 22      | 0     | 93568.906               | -0.473  | 34.5        | 199.9247                                             |                      |
| 23   | 2      | 22     | 1    | 23    | 1       | 22      | 0     | 101243.633              | 0.255   | 34.8        | 199.8015                                             |                      |
| 24   | 1      | 23     | 1    | 24    | 2       | 23      | 0     | 94677.029               | -0.489  | 39.6        | 213.4057                                             |                      |
| 24   | 2      | 23     | 1    | 24    | 1       | 23      | 0     | 100452.072              | 0.213   | 39.6        | 213.3128                                             |                      |
| 25   | 1      | 24     | 1    | 25    | 2       | 24      | 0     | 95546.737               | -0.525  | 39.4        | 227.4282                                             |                      |
| 25   | 2      | 24     | 1    | 25    | 1       | 24      | 0     | 99864.418               | 0.162   | 39.5        | 227.3587                                             |                      |
| 26   | 1      | 25     | 1    | 26    | 2       | 25      | 0     | 96230.704               | -0.509  | 44.1        | 241.9915                                             |                      |
| 26   | 2      | 25     | 1    | 26    | 1       | 25      | 0     | 99440.009               | 0.097   | 44.1        | 241.9398                                             |                      |
| 27   | 1      | 26     | 1    | 27    | 2       | 26      | 0     | 96770.969               | -0.500  | 44.0        | 257.0949                                             |                      |
| 27   | 2      | 26     | 1    | 27    | 1       | 26      | 0     | 99143.725               | 0.055   | 44.1        | 257.0567                                             |                      |
| 28   | 1      | 27     | 1    | 28    | 2       | 27      | 0     | 97200.941               | -0.513  | 48.5        | 272.7379                                             |                      |
| 28   | 2      | 27     | 1    | 28    | 1       | 27      | 0     | 98946.268               | 0.005   | 48.5        | 272.7099                                             |                      |
| 29   | 1      | 28     | 1    | 29    | 2       | 28      | 0     | 97546.875               | -0.509  | 48.6        | 288.9202                                             |                      |
| 29   | 2      | 28     | 1    | 29    | 1       | 28      | 0     | 98823.696               | 0.000   | 48.6        | 288.8996                                             |                      |
| 30   | 1      | 29     | 1    | 30    | 2       | 29      | 0     | 97828.953               | -0.479  | 52.8        | 305.6412                                             |                      |
| 30   | 2      | 29     | 1    | 30    | 1       | 29      | 0     | 98755.450               | 0.026   | 52.8        | 305.6264                                             |                      |
| 31   | 1      | 30     | 1    | 31    | 2       | 30      | 0     | 98060.635 <sup>c</sup>  | -0.690  | 53.0        | 322.9007                                             | B                    |
| 31   | 2      | 30     | 1    | 31    | 1       | 30      | 0     | 98713.724               | 0.195   | 52.9        | 322.8907                                             |                      |
| 32   | 1      | 31     | 1    | 32    | 2       | 31      | 0     | 98274.012               | 0.191   | 56.6        | 340.6980                                             |                      |
| 32   | 1      | 31     | 1    | 32    | 1       | 31      | 0     | 98614.669               | -0.963  | 0.5         | 340.6866                                             |                      |
| 32   | 2      | 31     | 1    | 32    | 2       | 31      | 0     | 98528.611               | 0.551   | 0.5         | 340.6980                                             |                      |
| 32   | 2      | 31     | 1    | 32    | 1       | 31      | 0     | 98869.244               | -0.626  | 56.0        | 340.6866                                             |                      |
| 33   | 1      | 32     | 1    | 33    | 2       | 32      | 0     | 98440.501               | -0.156  | 57.1        | 359.0339                                             |                      |
| 33   | 1      | 32     | 1    | 33    | 1       | 32      | 0     | 98643.608               | -0.556  | 0.3         | 359.0271                                             |                      |
| 33   | 2      | 32     | 1    | 33    | 2       | 32      | 0     | 98624.014               | 0.188   | 0.3         | 359.0339                                             |                      |
| 33   | 2      | 32     | 1    | 33    | 1       | 32      | 0     | 98827.119               | -0.214  | 57.0        | 359.0271                                             |                      |
| 34   | 1      | 33     | 1    | 34    | 2       | 33      | 0     | 98602.599               | -0.660  | 61.0        | 377.9074                                             |                      |
| 34   | 2      | 33     | 1    | 34    | 1       | 33      | 0     | 98881.092               | -0.001  | 61.1        | 377.9024                                             |                      |
| 35   | 1      | 34     | 1    | 35    | 2       | 34      | 0     | 98713.078               | 0.089   | 60.3        | 397.3186                                             |                      |
| 35   | 1      | 34     | 1    | 35    | 1       | 34      | 0     | 98833.538               | -0.150  | 1.3         | 397.3146                                             |                      |

TABLE 3—Continued

| $J'$ | $K'_a$ | $K'_c$ | $t'$ | $J''$ | $K''_a$ | $K''_c$ | $t''$ | Frequency<br>(MHz) | $O - C$ | $\mu^2 S^a$ | $E_{\text{lower}}$<br>( $\text{cm}^{-1}$ ) | Notes/<br>References |
|------|--------|--------|------|-------|---------|---------|-------|--------------------|---------|-------------|--------------------------------------------|----------------------|
| 35   | 2      | 34     | 1    | 35    | 2       | 34      | 0     | 98810.614          | 0.078   | 1.3         | 397.3186                                   |                      |
| 35   | 2      | 34     | 1    | 35    | 1       | 34      | 0     | 98931.034          | -0.201  | 60.3        | 397.3146                                   |                      |
| 36   | 1      | 35     | 1    | 36    | 2       | 35      | 0     | 98800.965          | 0.019   | 63.2        | 417.2683                                   | tg                   |
| 36   | 1      | 35     | 1    | 36    | 1       | 35      | 0     | 98935.903          | -0.224  | 2.2         | 417.2638                                   | tg                   |
| 36   | 2      | 35     | 1    | 36    | 2       | 35      | 0     | 98870.588          | 0.080   | 2.2         | 417.2683                                   | tg                   |
| 36   | 2      | 35     | 1    | 36    | 1       | 35      | 0     | 99005.484          | -0.206  | 63.3        | 417.2638                                   | tg                   |
| 37   | 1      | 36     | 1    | 37    | 2       | 36      | 0     | 99091.145          | 0.231   | 45.1        | 437.7481                                   | tg                   |
| 37   | 1      | 36     | 1    | 37    | 1       | 36      | 0     | 99033.377          | -0.319  | 20.5        | 437.7500                                   | tg                   |
| 37   | 2      | 36     | 1    | 37    | 2       | 36      | 0     | 99141.023          | 0.236   | 20.4        | 437.7481                                   | tg                   |
| 37   | 2      | 36     | 1    | 37    | 1       | 36      | 0     | 99083.254          | -0.316  | 45.4        | 437.7500                                   | tg                   |
| 38   | 1      | 37     | 1    | 38    | 2       | 37      | 0     | 99126.548          | -0.168  | 62.1        | 458.7733                                   | tg                   |
| 38   | 1      | 37     | 1    | 38    | 1       | 37      | 0     | 99145.500          | 0.056   | 7.4         | 458.7726                                   | tg                   |
| 38   | 2      | 37     | 1    | 38    | 2       | 37      | 0     | 99162.376          | -0.190  | 7.4         | 458.7733                                   | tg                   |
| 38   | 2      | 37     | 1    | 38    | 1       | 37      | 0     | 99181.326          | 0.032   | 62.2        | 458.7726                                   | tg                   |
| 39   | 1      | 38     | 1    | 39    | 2       | 38      | 0     | 99227.093          | -0.133  | 68.9        | 480.3330                                   |                      |
| 39   | 1      | 38     | 1    | 39    | 1       | 38      | 0     | 99242.045          | -0.093  | 1.1         | 480.3325                                   |                      |
| 39   | 2      | 38     | 1    | 39    | 2       | 38      | 0     | 99252.987          | -0.204  | 1.1         | 480.3330                                   |                      |
| 39   | 2      | 38     | 1    | 39    | 1       | 38      | 0     | 99267.951          | -0.152  | 69.0        | 480.3325                                   |                      |
| 40   | 1      | 39     | 1    | 40    | 2       | 39      | 0     | 99328.837          | -0.206  | 73.3        | 502.4292                                   |                      |
| 40   | 2      | 39     | 1    | 40    | 1       | 39      | 0     | 99359.031          | -0.383  | 73.3        | 502.4289                                   |                      |

NOTES.—(P) Predicted frequency with 300 kHz uncertainty; (B) blend; (gg) gauche + -gauche - interaction; (tg) trans-gauche interaction. See also Fig. 4.

<sup>a</sup> Units are Debye squared.

<sup>b</sup> Uncertainty of 150 kHz.

<sup>c</sup> Uncertainty of 100 kHz.

REFERENCES.—(1) Kakar & Quade 1980; (2) Cohen 1995.

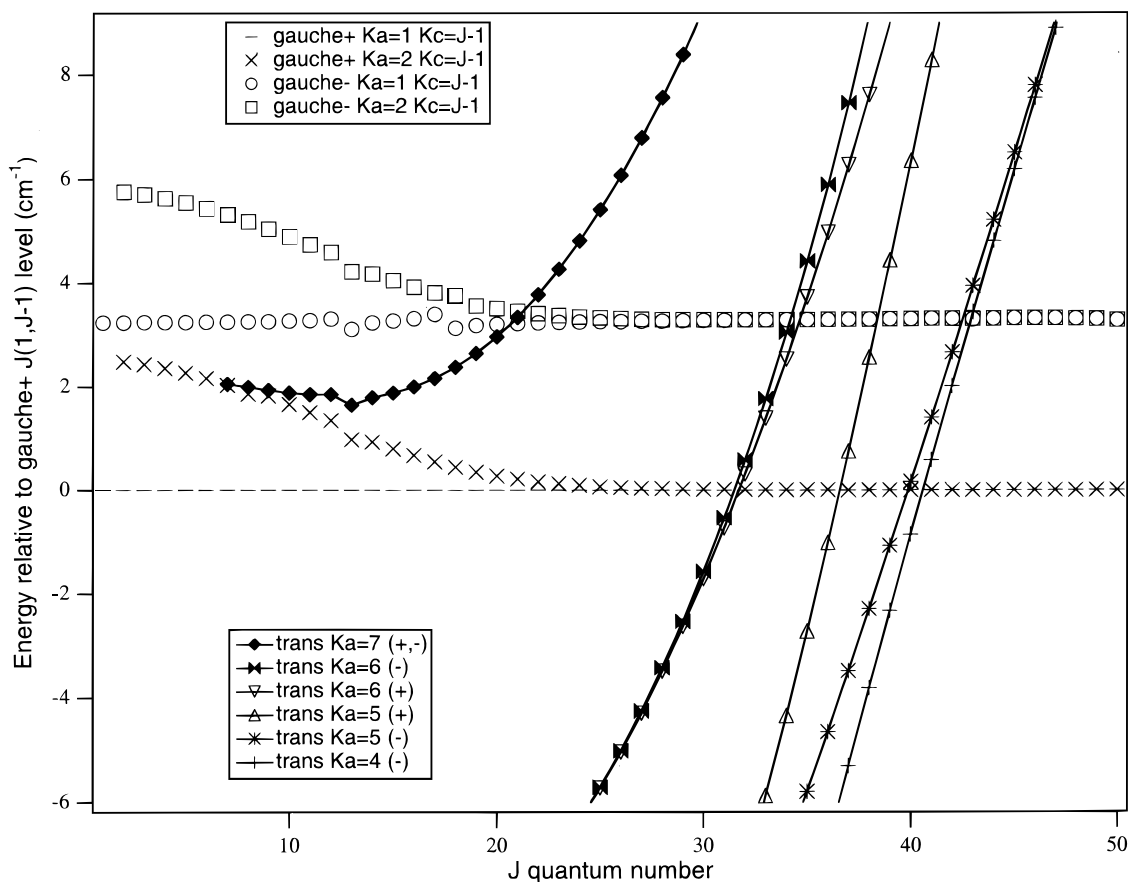


FIG. 4.—Crossings between two selected gauche+ and two selected gauche- rotational-torsional levels involved in the transitions analyzed here [ $J(1, J-1)$ ,  $J(2, J-1)$ ] with assorted rotational levels of the trans substrate. Energies relative to the lowest gauche rotational-torsional level of the four [gauche+;  $J(1, J-1)$ ] are plotted vs. total angular momentum quantum number  $J$ . At the crossings, perturbations which necessitate our current three-state analysis are at their maximum values. For a given series of rotational levels in the trans substrate, interactions occur either with the gauche+ or gauche- levels; these possibilities are indicated by + and -, respectively, in the labeling of the trans substrate series.

TABLE 4  
ORION-KL U-LINES ASSIGNED TO GAUCHE ETHANOL

| U-line<br>(MHz) | Laboratory Frequency<br>(MHz) | $T_A^*$<br>(K) | $\Delta v$<br>(km s <sup>-1</sup> ) | $\mu^2 S$<br>(D <sup>2</sup> ) | $E_{\text{upper}}$<br>(cm <sup>-1</sup> ) | $J'$ | $K'_a$ | $K'_c$ | $t'$ | $J''$ | $K''_a$ | $K''_c$ | $t''$ | $v_{\text{LSR}}$<br>(km s <sup>-1</sup> ) | Notes |
|-----------------|-------------------------------|----------------|-------------------------------------|--------------------------------|-------------------------------------------|------|--------|--------|------|-------|---------|---------|-------|-------------------------------------------|-------|
| U97536.9.....   | 97535.908                     | 0.08           | 4.3                                 | 45.60                          | 171.1318                                  | 21   | 1      | 21     | 1    | 21    | 0       | 21      | 0     | 6.0                                       | bl    |
| U97536.9.....   | 97536.849                     | 0.08           | 4.3                                 | 50.29                          | 195.7861                                  | 23   | 1      | 23     | 1    | 23    | 0       | 23      | 0     | 8.8                                       | bl    |
| U97547.3.....   | 97546.875                     | 0.06           | 3.0                                 | 48.54                          | 292.1740                                  | 29   | 1      | 28     | 1    | 29    | 2       | 28      | 0     | 7.7                                       |       |
| U97550.1.....   | 97549.692                     | 0.05           | 3.9                                 | 56.48                          | 236.8097                                  | 26   | 0      | 26     | 1    | 26    | 1       | 26      | 0     | 7.8                                       |       |
| U97563.2.....   | 97562.844                     | 0.05           | 2.6                                 | 51.78                          | 208.9221                                  | 24   | 1      | 24     | 1    | 24    | 0       | 24      | 0     | 7.9                                       |       |
| U97574.7.....   | 97574.042                     | 0.09           | 2.0                                 | 42.26                          | 159.6140                                  | 20   | 1      | 20     | 1    | 20    | 0       | 20      | 0     | 7.0                                       |       |
| U97597.8.....   | 97600.390                     | 0.21           | 2.7                                 | 54.95                          | 222.5973                                  | 25   | 1      | 25     | 1    | 25    | 0       | 25      | 0     |                                           | bl ex |
| U97632.2.....   | 97631.329                     | 0.06           | 2.9                                 | 59.59                          | 251.5631                                  | 27   | 0      | 27     | 1    | 27    | 1       | 27      | 0     | 6.3                                       |       |
| U97650.1.....   | 97649.502                     | 0.12           | 2.8                                 | 40.88                          | 148.6360                                  | 19   | 1      | 19     | 1    | 19    | 0       | 19      | 0     | 7.2                                       |       |
| U97756.4.....   | 97755.610                     | 0.05           | 2.5                                 | 61.17                          | 266.8558                                  | 28   | 1      | 28     | 1    | 28    | 0       | 28      | 0     | 6.6                                       |       |
| U97774.9.....   | 97774.307                     | 0.07           | 3.2                                 | 37.40                          | 138.1981                                  | 18   | 1      | 18     | 1    | 18    | 0       | 18      | 0     | 7.2                                       |       |
| U97816.8.....   | 97815.987                     | 0.05           | 2.7                                 | 64.11                          | 282.6859                                  | 29   | 1      | 29     | 1    | 29    | 0       | 29      | 0     | 6.5                                       |       |
| U97933.1.....   | 97932.445                     | 0.06           | 1.1                                 | 63.86                          | 315.9610                                  | 31   | 0      | 31     | 1    | 31    | 1       | 31      | 0     | 7.0                                       |       |
| U97963.2.....   | 97962.858                     | 0.09           | 1.5                                 | 36.11                          | 128.3004                                  | 17   | 1      | 17     | 1    | 17    | 0       | 17      | 0     | 8.0                                       |       |

NOTES.—(bl) blend; (ex) excluded from analysis.

the ground vibrational state (trans and gauche) up to  $J = 50$ . An analytical approximation to the three-substate  $Q_{\text{rs}}$ , accurate to within a few percent and based on the classical (continuous) approximation, is given by the expression

$$Q_{\text{rs}}(T) = T^{3/2} [3.27 + 3.34 \exp(-56.89/T) + 3.34 \exp(-61.54/T)] . \quad (4)$$

Interestingly, nuclear spin plays no role here because there is only one hydroxyl proton, so that Pauli exclusion principle considerations do not pertain, as long as motions in the remainder of the molecule cannot act in concert with the

hydroxyl proton to return the molecule to an indistinguishable configuration.

Figure 5 is the plot, known as a rotation diagram, for the transitions in Table 4. To produce the plot, unit beam efficiency has been assumed. The clearly blended line (U97597.8) has been excluded from the analysis. The U97536.7 blend has been included as an intensity weighted sum of the two transitions involved. From the 12 data points (11 single lines and one pair), we derive a best-fitting rotational temperature of  $223^{+66}_{-35}$  K, and a column density of  $2.8^{+3.9}_{-1.7} \times 10^{15} \text{ cm}^{-2}$ . With the proper beam efficiency of 0.40 (Ohishi et al. 1988), the column density rises to  $7.0 \times 10^{15} \text{ cm}^{-2}$ . Both the rotational temperature and the column density can be compared with the recent values of Ohishi et al. (1995), determined from an analysis of four low-lying lines of trans-ethanol. These authors obtained a rotational excitation temperature of 70 K, which is significantly lower than our result. Using their temperature to determine the ratio of the total to trans partition functions, we calculate that their column density should be multiplied by a factor of  $\approx 2$  to obtain a total column density. With the higher temperature, a factor of  $\approx 3$  is more applicable. The resulting total column density of  $2\text{--}3 \times 10^{15} \text{ cm}^{-2}$  is in reasonable agreement with our value. Although the rotational temperature we obtain is not in good agreement with that of Ohishi et al. (1995), it is in better agreement with an earlier value of Turner (1991) who determined a rotational temperature of 216 K for trans-ethanol with a-type transitions neglected.

TABLE 5  
ROTATIONAL PARTITION FUNCTION  
FOR ETHANOL

| Temperature<br>(K) | $Q_{\text{rs}}^a$ | $\log_{10}(Q_{\text{rs}})$ |
|--------------------|-------------------|----------------------------|
| 9.375 .....        | 95.5968           | 1.9804                     |
| 18.570 .....       | 290.9459          | 2.4638                     |
| 37.500 .....       | 1072.4158         | 3.0304                     |
| 75.000 .....       | 4106.3917         | 3.6135                     |
| 150.000 .....      | 14299.1626        | 4.1553                     |
| 225.000 .....      | 28161.6572        | 4.4497                     |
| 300.000 .....      | 44151.7878        | 4.6449                     |

<sup>a</sup> Explicit sum over all ground state rotational torsional levels (trans, gauche+, and gauche-) through  $J = 50$ ,  $K_a = 50$ .

TABLE 6  
ADDITIONAL PROPOSED ASSIGNMENTS

| U-line<br>(MHz) | $J'$ | $K'_a$ | $K'_c$ | $t'$ | $J''$ | $K''_a$ | $K''_c$ | $t''$ | Laboratory Frequency<br>(MHz) | $v_{\text{LSR}}$<br>(km/s) | $T_R/T_A^*$<br>(K) | Reference | Source   |
|-----------------|------|--------|--------|------|-------|---------|---------|-------|-------------------------------|----------------------------|--------------------|-----------|----------|
| U78640.....     | 5    | 0      | 5      | 1    | 5     | 1       | 5       | 0     | 78637.457                     | -1                         | 0.05               | 1         | Orion-KL |
| U90355.....     | 21   | 1      | 20     | 1    | 21    | 2       | 20      | 0     | 90354.336                     | 7                          | 0.08               | 1         | Orion-KL |
| U97263.....     | 23   | 0      | 23     | 1    | 23    | 1       | 23      | 0     | 97263.540                     | 10                         | 0.01               | 1         | Orion-KL |
| U98230.2.....   | 16   | 1      | 16     | 1    | 16    | 0       | 16      | 0     | 98230.313                     | 9.1                        | 0.02               | 2         | Orion-KL |
| U99142.....     | 27   | 2      | 26     | 1    | 27    | 1       | 26      | 0     | 99143.725                     | 14                         | 0.10               | 1         | Orion-KL |
| U100453.....    | 24   | 2      | 23     | 1    | 24    | 1       | 23      | 0     | 100452.072                    | 59                         | 0.08               | 1         | Sgr B2   |
| U102490.....    | 11   | 1      | 11     | 1    | 11    | 0       | 11      | 0     | 102489.386                    | 7                          | 0.03               | 1         | Orion-KL |
| U103796.....    | 10   | 1      | 10     | 1    | 10    | 0       | 10      | 0     | 103796.950                    | 12                         | 0.02               | 1         | Orion-KL |

REFERENCES.—(1) Turner 1989; (2) Kutner et al. 1980.

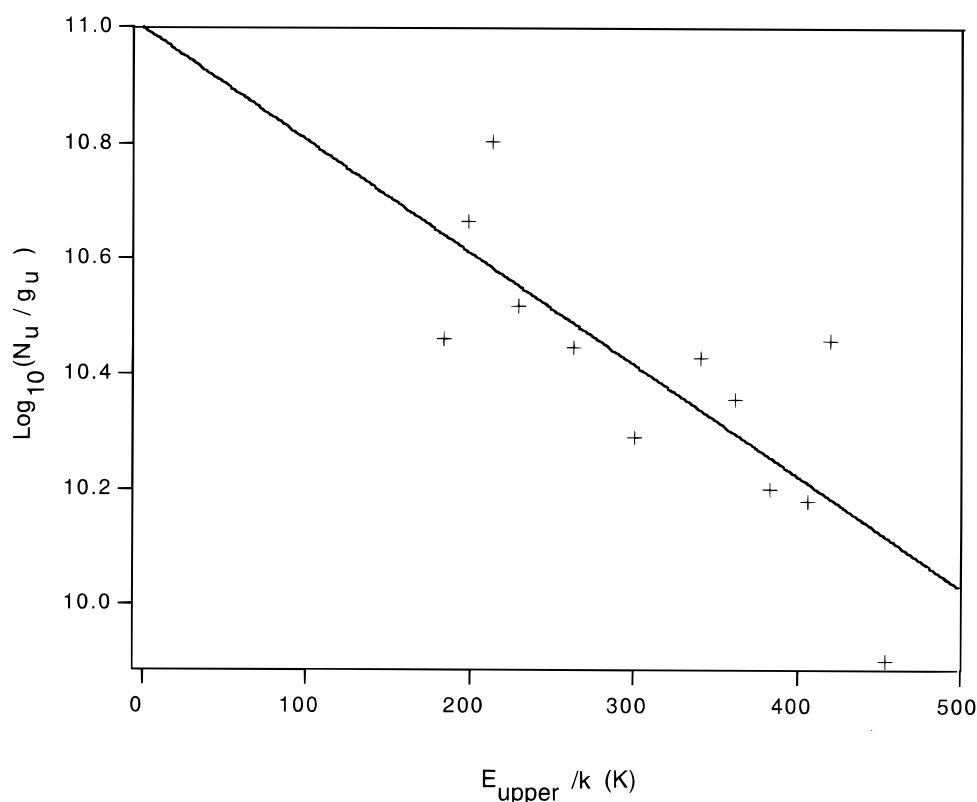


FIG. 5.—Rotation diagram for ethanol in Orion KL using the measured  $U$  lines of Ohishi et al. (1988)

It is interesting to speculate on whether the Orion KL  $U$  lines assigned here belong to the Hot Core or to the Compact Ridge. The latter source is known for oxygen-containing organic molecules, although many molecules in this source have lower rotational temperatures than we determine for gauche ethanol. The  $v_{\text{LSR}}$  values and line-widths in Table 4 indicate that gauche ethanol lies in the Compact Ridge (Ohishi 1996). It also seems clear that the trans-ethanol lines seen by Ohishi et al. (1995) stem from the Compact Ridge. Assuming ethanol to lie in either the Hot Core or the Compact Ridge, its fractional abundance with respect to  $\text{H}_2$  can be estimated to be  $\approx 1\text{--}2 \times 10^{-8}$ , a number equivalent to that determined for other sources, and only an order of magnitude or so below that of methanol.

Table 6 contains a second list of  $U$  lines reported by Lovas (1991) that may be attributable to the gauche ethanol  $Q$ -branch transitions presented in this paper. In addition to the  $U$  lines and relevant laboratory ethanol frequencies, Table 6 includes proposed assignments, astronomical sources,  $T_R/T_A^*$ ,  $v_{\text{LSR}}$  values, and the original references for the  $U$  lines. The lines are, with one exception, reported to only 1 MHz ( $3 \text{ km s}^{-1}$ ), so that  $v_{\text{LSR}}$  information is not very precise. Still it can be seen that our assignments for U78640 and U99142 are the least likely, since their estimated  $v_{\text{LSR}}$  values are well outside the  $5\text{--}8 \text{ km s}^{-1}$  range of Orion KL.

## 5. SUMMARY

This is the third paper in a series on the laboratory millimeter-wave and submillimeter-wave spectrum of ethanol. In this paper, we introduce for the first time an analysis in which interactions among the three torsional

substates of the ground vibrational state are considered. Without a consideration of these interactions, previous separate analyses of the lowest trans substate (Pearson et al. 1995) and the excited gauche substates (Pearson et al. 1996) are limited to a restricted range of angular momentum quantum numbers. Although our three-substate analysis is currently capable of fitting 3500 transitions to a root mean square deviation of 400 kHz, we anticipate that future improvements will permit us to fit the laboratory data to near experimental accuracy (50–100 kHz). At the current stage of development, we have successfully analyzed four often badly perturbed gauche—gauche+  $Q$ -branches. In addition, we have been able to predict line positions and calculate intensities for a large number of other perturbed transitions. Finally, the trans—gauche+ energy difference of  $1185399.1 \pm 5.0 \text{ MHz}$  has been accurately determined.

From our measurements and calculations, we have assigned 14 astronomical  $U$  lines in the 97.5 to 98.0 GHz region of the spectrum, seen in the direction of Orion KL, to transitions between the two gauche substates of ethanol. Analysis of these lines indicates a high rotational temperature (223 K) and a large ethanol column density ( $7.0 \times 10^{15} \text{ cm}^{-2}$ ) representative of a hot core-type source, most probably the Compact Ridge. The rotational temperature is approximately a factor of 3 larger than that determined using low-lying transitions in trans-ethanol by Ohishi et al. (1995) in the Compact Ridge. Perhaps one temperature does *not* describe the rotational torsional distribution of ethanol towards Orion KL.

Whatever its temperature, the large abundance of ethanol cannot be accounted for purely by gas-phase chemistry, indicating yet again the importance of dust chemistry in the

formation of saturated interstellar organic molecules. We have also proposed assignments for eight additional interstellar *U* lines to our recently analyzed gauche— to gauche+ *Q*-branch ethanol transitions. Two of these assignments are ambiguous. Other tentative assignments of *U* lines in Sgr B2 and other sources to gauche ethanol based on our original work (Pearson et al. 1996) have been communicated to us by Millar (1996) and Ohishi (1996).

Previous determinations of interstellar column densities for ethanol have, to the best of our knowledge, ignored the gauche substates. Since these substates comprise two thirds of the ground vibrational state energy levels, they must be considered in column density determinations, unless the excitation temperature is considerably lower than the 57 K excitation of the gauche+ substate. Because ethanol appears to be abundant only in warmer regions of molecular clouds, this exception is unimportant.

A machine-readable list of ethanol frequencies and intensities based on our work can be found in the JPL Submillimeter, Millimeter, and Microwave Spectral Line Catalog (Poynter & Pickett 1985; Pickett et al. 1996; available online at <http://spec.jpl.nasa.gov>). The list is being updated. The intensities  $I$  ( $\text{nm}^2 \text{ MHz}$ ) in the JPL catalog, based on integrated cross sections at 300 K, have to be converted to  $\mu_x^2 {}^xS_{ba}$  for astronomical use. A general conversion formula is

$$\mu_x^2 {}^xS_{ba} = \frac{I \times 2.403 \times 10^4}{\nu_{ba}} \times \frac{1}{\exp(-E_l/208.5) - \exp(-E_u/208.5)} Q_{rs}(300 \text{ K}) \quad (5)$$

where the frequency  $\nu_{ba}$  is in MHz, the upper and lower state energies  $E_u$  and  $E_l$  are in  $\text{cm}^{-1}$ , and  $\mu_x^2 {}^xS_{ba}$  is in units of Debye<sup>2</sup> (1 Debye =  $10^{-18}$  esu cm).

The portion of this work performed at the Jet Propulsion Laboratory, California Institute of Technology, was done under contract with the National Aeronautics and Space Administration. We would like to thank NASA for their support of laboratory astrophysics at the Ohio State University and the Ohio Supercomputer Center for the award of time on their Cray YMP8 computer. K. V. L. N. Sastry thanks Deutscher Akademischer Austauschdienst (DAAD) for financial support during his stay in Giessen, Germany. The laboratory work in Giessen was supported by the Forschungsgemeinschaft and Fonds der Chemischen Industrie. Special thanks are due to Masatoshi Ohishi for his criticism of an earlier version of this manuscript and for his help with our foray into radio astronomy.

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