THE SUBMILLIMETER-WAVE SPECTRUM OF ISOTOPIC METHYL CYANIDE

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1 The research was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract with the National Aeronautics and Space Administration.
ABSTRACT

The laboratory submillimeter-wave rotational spectrum of the $^{13}$CH$_3$CN, CH$_3^{13}$CN, and the CH$_3$C$^{15}$N isotopomers of methyl cyanide has been observed in natural abundance in the 294 to 607 GHz region. The maximum J and K values are 34 and 14, respectively. Fifteen additional CH$_3$CN transitions up to K=21 were also measured. The transitions of all four species are fitted to a symmetric top Hamiltonian and the rotation and distortion constants are determined. The $^{14}$N quadrupole and spin rotation coupling constants are also calculated and presented. Suggested values for many other parameters which could not be directly determined from the isotope spectra are calculated from the normal species values and isotope relationships. The determined and calculated constants should predict the spectrum of the three isotopomers to well over 1 THz accurately enough for astronomical assignments.

Subjectheadings: interstellar molecules - laboratory spectra - line identification - molecular processes
1. INTRODUCTION

Methyl cyanide or acetonitrile is a well-known interstellar molecule with densities in some sources exceeding 1 x 10^6 cm^-3 (Sutton et al. 1986). The normal species was first detected in the interstellar medium by Solomon, Jefferts, Panzias, & Wilson (1971). Since that time rotational transitions of the two singly substituted ^{13}C isotopes (Cummins et al. 1983 and Sutton et al. 1985), the 365.015965(12) cm^-1 (Koivusaari, Horneman, & Antila 1992) ν_b=1 bending state of CH_3CN (Goldsmith et al. 1983), and the CH_2DCN species (Gerin et al. 1992) have been observed. Methyl cyanide has been detected in nearby galaxies (Mauersberger et al. 1991) and used to make maps of star forming regions (e.g. Habing & Macdonald 1991 and Olmi, Cesaroni, & Walmsley 1993). Rotational temperatures of over 200 Kelvin (e.g. Sutton et al. 1986) have been reported in some hot cores. At such high temperatures, CH_3CN significantly populates states which have transitions far into the submillimeter region. The rapid development of very sensitive receivers working far into the submillimeter and their use in surveys of hot sources has provided an urgent need to extend the range of quantum numbers where species known to exist in these sources can be accurately predicted.

Methyl cyanide is a textbook example of a prolate symmetric top featuring a large dipole moment, μ_0 = 3.92197 (13) Debye (Gadh et al. 1995) and μ_0 = 3.9256(7) for CH_3C^{15}N (Mite, Sakai, & Katayama 1984). Since it is a symmetric top (C_3v symmetry), it features closely spaced transitions at very different energies in two distinct non-interacting symmetries A and F; with K=3n and K≠3n (n=0, 1, 2, 3...), respectively. The high abundance of CH_3CN and its symmetric top spectral pattern makes it an excellent probe of temperature and excitation in a number of regions (e.g. Cummins et al. 1983, Loren & Mundy 1984, Sutton et al. 1986, and Bishop 1990). The relative abundance of the A and F: symmetries has also been a subject of interest (e.g. Sutton et al. 1986). The transitions of the CH_3^{13}CN species closely track the normal species with the K=0 transitions in the submillimeter typically appearing near the K=6 normal species transition.
The 1T113~N and the CH3C\(^{13}\)N species have transitions appearing in the same spectral regions but are well separated from the normal species due to their smaller \(B\) rotational constants.

Methyl cyanide was one of the first molecules studied with microwave spectroscopy (Ring et al. 1947). A thorough summary of investigations before 1980 was published by Boucher et al. (1980). Between 1980 and now the normal species measurements were extended well into the submillimeter with a variety of techniques (Bocquet et al. 1988, Pavone et al. 1990, Carlotti, DiLeonardo, & Fusina 1988, and Brown, Dangoisse, & Demaison 1988). With the exception of some Russian work without published transition frequencies, CH\(_2\)DCN was the only isotope to be studied in the submillimeter region (Le Guennec et al. 1992) and subsequently observed (Gerin et al. 1992). In this paper, we report submillimeter measurements of the \(^{13}\)CH\(_3\)CN, CH\(_3\)\(^{13}\)CN and 013~1 'N isotopomers, in addition to the isotopic species we report a thorough analysis of the normal species including a few new high \(K\) transitions. The higher order 013C~N parameters are used in conjunction with isotope relations to derive a suggested set of higher order constants for the isotopic species. Predictions through \(J=99\) for methyl cyanide and its isotopomers are too lengthy to publish here, but they are available on-line from the JPL spectral line catalog at spec.jpl.nasa.gov or by anonymous ftp at the same site.

2. EXPERIMENTAL

The sample of CH\(_3\)CN was obtained commercially from Matheson, Coleman, and Bell and required no further purification. Measurements were made with tone burst modulation on 100 GHz phase locked klystrons driving point contact harmonic generators. Second derivative detection using a 4.2 K InSb hot electron bolometer was employed. The data were digitized directly by a computer for further analysis. Measurements were made at room temperature in a double pass polarization rotating one meter cell. The details of this
spectrometer system are described elsewhere (Triedl et al. 1995). All measurements were made in natural isotopic abundance at pressures of 1-10 milli-torr. Higher pressures resulted in excessive pressure broadening due to the large dipole moment. Measurement accuracy is estimated to be 30 kHz for the strongest low K transitions up to 150 kHz for the weakest transitions.

Initial predictions for the three isotopic species were based on an analysis of the data in Boucher et al. (1980). These predictions facilitated rapid assignment of the observed spectra in the 290 to 442 GHz region. The 606 GHz transitions were predicted with the aid of the newly measured transitions and were once again readily assignable. Initial normal species predictions were the result of an analysis of the existing data discussed in the following section. As expected, only small deviations within the predicted uncertainty from the initial line positions were observed at the highest K values.

3. ANALYSIS

The CH$_3$CN analysis used the data in Boucher et al. (1980), Pavone et al. (1990), Bocquet et al. (1988), Kukolich et al. (1978), and Kukolich (1982) along with the 15 newly measured transitions reported in Table 1. The lower resolution measurements from a variety of sources were not included in the analysis. The transitions reported in Kukolich et al. (1978, 1981) with resolved hydrogen hyperfine were averaged according to relative intensities into $^{14}$N quadrupole hyperfine components. The $^{13}$CH$_3$CN analysis used transitions reported in Boucher et al. (1980) and the 55 new measurements reported in Table 2. The J=1$\leftrightarrow$0 transition was measured at the University of British Columbia with a Fourier transform microwave spectrometer described in (Xu, Jäger, & Gerry 1992).

The, CH$_3^{13}$CN analysis used the transitions reported in Boucher et al. (1980), Kukolich et al. (1978, 1982) and the 39 new measurements reported in Table 3. The measurements of Kukolich et al. (1978, 1981) appear to be slightly less precise than in the normal species due to the additional complication of the $^{13}$C spin. The J= 1$\leftrightarrow$0 transition
was re-measured at the University of British Columbia and was in excellent agreement with the Kukolich et al. (1978) measurements used in the analysis. The CH$_3$C$^{15}$N analysis used transitions reported in Boucher et al. (1980) and the 37 newly measured transitions in Table 4. The J=1→0 transition was measured at the University of British Columbia. In addition to the transitions, Tables 1 through 4 include the fitted observed minus calculated, the lower state energy in wavenumbers, and the log base 10 of the line intensity at 300 K, $I_{300}$, in units of mm$^2$ MHz. The line intensity at temperature ‘1’ is given by

$$ I(T) = (8\pi^3/3h\nu) v_{nu} \cdot s_{nu}/[e^{-E/kT} - \frac{E/kT}{1 + Q_{rs}}], $$

where $v_{nu}$, $s_{nu}$, $\mu_x$, $E''$, $E'$, and $Q_{rs}$ are the transition frequency, line strength including the 2:1 A to I; statistics, the dipole component along the x axis, lower and upper state energies, and the rotation-spin partition function. For brevity, the line intensities given are a sum of all K parity transitions and the major hyperfine components unless resolved. The partition functions $Q_{rs}$ are given explicitly for each isotopomer. Here are additional low J transitions for all the isotopomers reported in the literature; however, they were found to be of lower resolution and contained no new information.

The analysis included the effects of $^{14}$N quadrupole and the spin rotation coupling where resolved, but none of these effects were observed in the submillimeter region. The CH$_3$CN lines did appear to broaden somewhat at K near J but no splittings could be resolved. The normal species ground state rotation and distortion constants determined were B, D$_J$, D$_{JK}$, H$_J$, I$_{JK}$, I$_{KJ}$, I$_{JJK}$, I$_{JJK}$, and I$_{JJK}$. The rotation and distortion constants determined for the three isotopic species were B, D$_J$, D$_{JK}$, I$_{JK}$, and I$_{KJ}$. The rotation and distortion constants along with the $^{14}$N quadrupole ant] spin rotation constants derived from the fit are given on Table 5. Additional constants were fixed to the normal species values and are discussed in the following section.

4. DISCUSSION
The rotational constants $A$, $D_K$ and $I_J K$ cannot be determined from the existing microwave spectra and in general cannot be determined from microwave spectra in $C_3v$ molecules without the aid of a suitable resonance; however, these values are needed to calculate relative intensities and rotational energies. As a result, it is necessary to use the $A$, $D_K$ and $I_J K$ values determined from the infrared spectroscopy of the $v_8$, $v_7+v_8$, and $v_7+v_8$ bands (Anttila et al. 1993). The $A$ values given in Table 5 for the isotopic species were calculated by scaling the measured normal species $A$ value by the ratio of $A_n/A_i$ ($n=$ normal, $i=$ isotopomer) obtained from the ground state average ($r_2$) structure which accounted for isotope effects on bond lengths determined by Demaison et al. (1979). The measured $D_K$ constants for the normal species were scaled by the ratio of the $A$'s squared. The $I_J K$ constants were not scaled since the scaling is small compared to the uncertainty in this parameter.

In order to generate accurate predictions to over a THz, the $I_J$ values for $^{13}$CH$_3$CN and CH$_3$C$^{15}$N were calculated by scaling the normal species value by the ratio of the $D_J$ constants to the $3/2$ power. The CH$_3^{13}$CN$I_J$ value was fixed to the ground state since the $D_J$'s were approximately equal. The values of the $I_{JJK}$, $I_{JK}$, and $I_{JKK}$ constants are determined for the normal species, but only $I_{JJK}$ has a significant effect on the fit. These constants were included to give a more realistic prediction of the transition frequency uncertainty in the normal species and the transition frequencies in the isotopomers at higher $J$ and $K$ values. Since the values of these parameters are not particularly well determined, the isotopic species $I$ constants were fixed to the normal species values.

The uncertainty in the $C_3-C_1$ spin rotation parameter in CH$_3$CN was greatly affected by the uncertainty assigned to the lowest $J$ transitions; however, the value was relatively independent of the uncertainties used. In all the weighting schemes tried, the value varied at most 25% of its quoted uncertainty. The $C_3-C_1$ spin rotation parameter could not be determined in either of the two $^{13}$C isotopomers and was fixed to the main
isotope, The $^{14}$N quadrupole was well determined for all three isotopomers containing $^{14}$N. The $C_4$ parameter was determined for the main isotope and the two $^{13}$C isotopes. The values of the constants determined should predict the spectrum of $^{13}$CH$_3$CN, CH$_3^{13}$CN, and CH$_3^{15}$N to well over 1 THz with the accuracy required to assign interstellar spectra.

Acknowledgment

11. S. P. M. thanks the National Research Council for a NRC-NASA Resident Research Associateship. We also thank Bethany Gatehouse and Dr. Thomas Brupbacher at the University of British Columbia for making their measurements of the $J=1 \leftarrow 0$ transitions available.
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\*a\ See text. The partition function to \( J=99 \) including the \( v_8=1 \) state and the \( ^{14}N \) quadrupole multiplicity is \( Q_{J'=99} = 41077.6558 \).

\*b \( \lambda \) energy of the lower state.
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a See text. The partition function to J=99 including the 14N quadrupole multiplicity is Q_J=3 1255.7298.
b Total energy of the lower state.

Note: F' quantum numbers given only if resolved.
### Table 3
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(a) See text. The partition function to $J=99$ including the $^{14}$N quadrupole multiplicity is $Q_{rs}=30370.2787$.

(b) Total energy of the lower state.
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a See text. 'l' repartition function to J=99 is Qₗₙ=10431.6539.
b Total energy of the lower state.
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<th>$^{13}$CH$_3$CN Value$^a$ (MHz)</th>
<th>CH$_3^{13}$CN Value$^a$ (MHz)</th>
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<td>B</td>
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$^a$ One standard deviation in units of last decimal place given.
$^b$ Fixed value from Anttila et al. (1993).
$^c$ Fixed calculated value see text.
$^d$ Fixed value from Gadhi et al. (1995).
$^e$ Fixed value from Mite, Sakai, & Katayama (1984).
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Xu, Y., Jäger, W., & Gerry, M. L. C., 1992, J. Mol. Spectrosc. 151, 206