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Far infrared spectrum of Methanol-D_2 in the lowest torsional state (e_0)

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HIGHLIGHTS

- Infrared Spectral Transitions in the torsional ground state CHD_2OH observed.
- Assignments are confirmed by combination loops.
- The results will be useful for Astronomical and laser discovery.
- Corroborate MMW spectral study.
- *Further work is in progress.*

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ABSTRACT

The infrared (IR) and far infrared (FIR) absorption spectra have been measured for the Methanol-D_1 and D_2 species in the wave number range of 20–1200 cm^{-1} at the Justus Liebig Universität in Giessen, Germany using a Brüker Fourier Transform spectrometer at a resolution of 0.002 cm^{-1}. The spectra looked very complicated but analyses were possible for the lower lying states. At higher wave number regions spectra of few vibrational fundamental modes were visible. In this communication, the details of the assignments and analyses of the lowest lying internal rotational state (e_0) for Methanol-D_2 are reported. A catalog of about 900 assigned spectral lines has been prepared and is made available from the author to conserve space. As application of this work, it was possible to assign some optically pumped FIR laser lines to quantum states. The results should be useful for "radio astronomers" and in the field of optically pumped FIR and Sub-millimeter Wave (SMMW) lasers which are used in Tokamaks for plasma diagnostics and as local oscillators in radio detection from space.

1. Introduction

The Fourier Transform Infrared (FTIR) Spectral technique is an indispensable tool for the characterization of internal energy levels of complex molecules. In recent years there have been a renewed interest in the study of methanol and its isotopic variants in the IR regions mainly because of the ability of these molecules to emit lower frequency laser lines when optically pumped by the 10 μm CO_2 lasers [1–7]. The spectroscopy of the asymmetrically deuterated methanol species poses a real challenge to scientists because the internal potential barrier to internal rotation in the molecule is not clearly 3-fold symmetric about the quasi-symmetry axis of the molecule. This introduces the internal rotational vibrational (torsional) states to be highly mixed thereby making the selection rules for transitions quite relaxed and hence making the spectra very crowded and complex to decipher. This deterred the study of the internal energy structure of these molecular species. The FTIR spectroscopy has proved to be a powerful tool in this process not only because of large range of coverage of the spectra but also the high precision of the frequencies of spectral lines obtained by using a large path length in the absorption process. The repeatability and stability of the commercial FTIR instruments allow addition of a large number of scans and improve the signal to noise (S/N) ratio and to measure weak feathers in the spectra. The ability of lowering the temperature of the gas sample also simplifies the spectra by increasing the population of lower lying states.

The spectra were recorded at two different temperatures at a nominal resolution of 0.002 cm^{-1}. The spectra recorded earlier for rotational transitions in the millimeter wave (MMW) region [8,9] were mutually beneficial for the assignment scheme. The results should find applications to the identification of these molecular species in interstellar space [10,11] and in the field of optically pumped molecular lasers.

The off-axis substituted deuterium CHD_2OH results the hindering internal rotational potential to lift the 3-fold symmetry. This removes the degeneracy of the three possible sublevels

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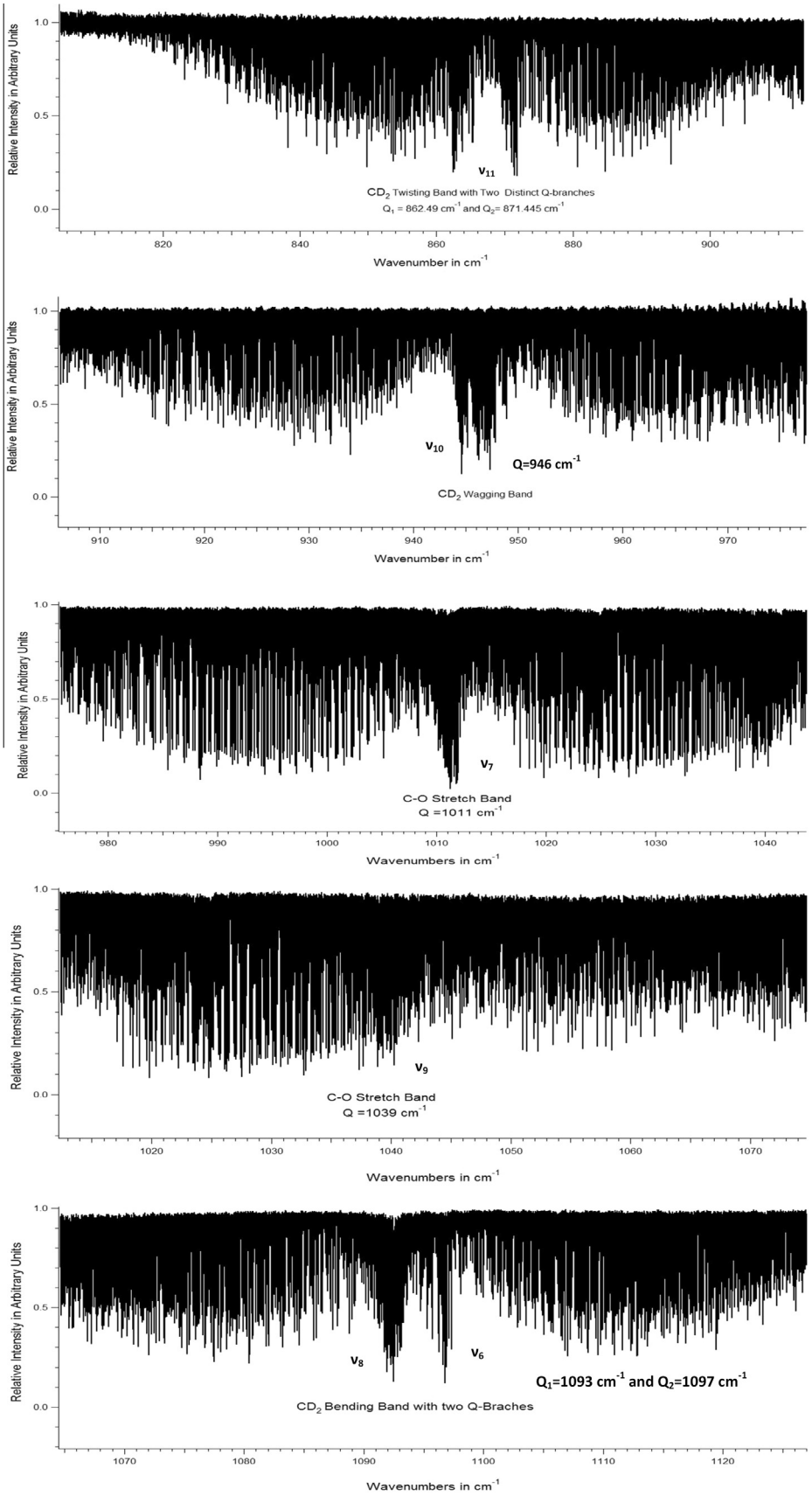

Fig. 1. The vibrational fundamental bands of Methanol-D_2 recorded in this work.