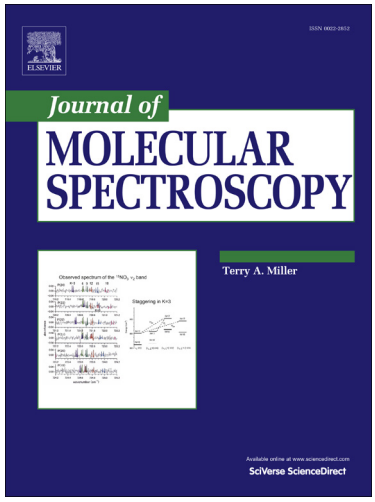

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The rotational spectrum of methyl ethyl ketone in its ground vibrational state

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Abstract

The molecule 2-butanone, or methyl ethyl ketone (MEK), $CH_3COCH_2CH_3$, has been studied from 8 GHz – 1 THz using a combination of chirped-pulse Fourier transform microwave spectroscopy and direct absorption millimeter/submillimeter spectroscopy. This molecule is of interest for the field of astrochemistry because it has functional groups in common with several known interstellar molecules, and therefore could serve as a tracer of grain surface formation pathways for complex organics in interstellar clouds. The results of the spectral studies and the analysis of the ground vibrational state of methyl ethyl ketone up to 1 THz are presented here. The challenges of spectral analysis for an organic molecule with spectral complexity arising both from internal rotation and many low-lying vibrational states are discussed. The performances of several standard fitting packages are compared in terms of handling this challenging spectral analysis problem.

Keywords: 2-butanone; rotational spectroscopy; chirped-pulse spectroscopy; broadband spectroscopy; microwave spectroscopy

1. Introduction

The molecule 2-butanone, or methyl ethyl ketone (MEK), $CH_3COCH_2CH_3$, is a common industrial solvent. MEK is of interest for interstellar chemistry because it contains the methyl, ethyl and carbonyl functional groups, which are found in a variety of complex organic molecules (COMs) observed in star-forming regions. COMs are thought to form through a combination of condensed-phase radical-radical reactions on interstellar grains in cold regions, and gas-phase ion-molecule reactions in warm regions [1]. Examination of the spatial distributions of a set of molecules containing the same functional groups could reveal important information pertaining to the chemical mechanisms at play in interstellar regions, as molecules with similar formation and destruction pathways would be expected to be cospatial in a given interstellar source [2]. MEK therefore could serve as a probe of radical-radical addition reactions involving methyl and ethyl groups with carbonyl-containing molecules. Other previously detected COMs that have functional groups in common with MEK include methanol (CH_3OH), ethanol (CH_3CH_2OH), dimethyl ether (CH_3OCH_3), acetone (CH_3COCH_3), methyl formate ($HCOOCH_3$), acetaldehyde (CH_3CHO), and propanal (CH_3CH_2COH). The chemistry involving these and other molecules that are commonly found in interstellar environments is reviewed by Herbst and van Dishoeck [3], and further information can be found in that review and references therein.

MEK is a stable molecule that is a liquid at room temperature. The high MEK vapor pressure combined with dipole moment components of μ_a=0.079 D and μ_b=2.778 D [4] make collection of its spectrum straightforward. MEK has two terminal methyl groups that can undergo internal rotation. The methyl group closest to the carbonyl has a V_3 barrier to internal rotation of 183 cm^{-1} [4], while the group furthest from the carbonyl has a V_3 barrier to internal rotation of 795 cm^{-1} [5]. Previous laboratory studies have been performed in both the microwave [4, 5] and the infrared regions [6], with the microwave work including the range of 9 to 33 GHz. The work of Pierce et al. [4] focused on the rotational spectrum of the ground vibrational state, and included treatment of effects that arose due to the rotation of the methyl group nearest to the carbonyl bond. The work of Pozdeev et al. [5] involved analysis of the rotation of the methyl group furthest from the carbonyl bond, and the first excited state of the torsional vibration about the central C-C bond. Neither of these previous studies report spectral evidence of the high energy conformer (*cis*-MEK). The barrier to rotation about the central C-C bond was found to be 5500 cm^{-1} [5]. Therefore, the strongest lines in the rotational spectrum of MEK at room