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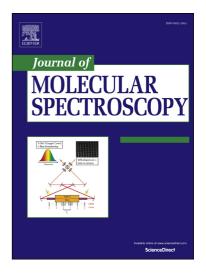
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Millimeter and Submillimeter Spectrum of Propylene Oxide

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Abstract

The spectrum of propylene oxide was collected from 70 GHz to 1 THz using direct absorption millimeter and submillimeter spectroscopy. Analysis of the spectrum was performed using the SPFIT/SPCAT programs for the A state. A full internal rotor analysis was performed using the XIAM program. The barrier to internal rotation of the methyl group was determined to be 893 cm⁻¹. The precision of the rotation constants, centrifugal distortion constants, and internal rotor parameters was increased over the results reported by previous low-frequency studies. The results of this laboratory study and the associated analysis, as well as a spectral prediction for the ground vibrational state of propylene oxide, are presented.

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Keywords: Propylene Oxide, mm/submm spectroscopy, internal rotation

1. Introduction

One of the most curious and elegant phenomena of molecular biology is nature's selection of specific enantiomers of chiral molecules, molecules that are non-superimposable mirror images of one another. For life on Earth to exist as it does today, it was a necessity for the biochemical makeup of organisms to develop homochirality, or chiral homogeneity [1]. One example is amino acids, the building blocks of proteins. The amino acids we know to exist in living organisms are of the L-type enantiomer, though the R-type enantiomer is of equal physical properties [2]. Several mechanisms have been proposed to elucidate the propagation and amplification of homochirality, usually by assuming a low initial enantiomeric excess (e.e.) [3, 4]. The particularly quizzical problem is how an e.e. comes to exist out of nature when chiral enantiomers share the same chemical properties. Biochemists believe this process to have occurred from a racemic mixture of chiral molecules in a system of such complexity as an early Earth [3]; however, studies of chiral molecules in meteorites have shown an e.e. to exist in the Murchison meteorite [5]. A number of laboratory studies have shown that it is possible to amplify an e.e. in solution by exposure to circularly polarized light [6, 7]. While it is possible that chemistry occurring in these meteorites could have potentially created an e.e., it is also possible that the excess was created in the birth place of both meteorites and Earth: interstellar molecular clouds. If an e.e. could be formed in a molecular cloud, it could be inherited and amplified by its descendants meteorites, comets, and planets alike. Studying chiral molecules in molecular clouds can give great insight into the origin of homochirality.

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