

238

Accession number:20114914583124

Title:Terahertz spectroscopy of isotopic acrylonitrile

Authors:Krasnicki, Adam (1); Kisiel, Zbigniew (1); Drouin, Brian J. (2); Pearson, John C. (2)

Author affiliation:(1) Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland; (2) Jet Propulsion Laboratory, California Institute of Technology, 4800 Oak Grove Drive, Pasadena, CA 91109-8099, United States

Corresponding author:Kisiel, Z.(kisiel@ifpan.edu.pl)

Source title:Journal of Molecular Structure

Abbreviated source title:J. Mol. Struct.

Volume:1006

Issue:1-3

Issue date:December 14, 2011

Publication year:2011

Pages:20-27

Language:English

ISSN:00222860

CODEN:JMOSB4

Document type:Journal article (JA)

Publisher:Elsevier, P.O. Box 211, Amsterdam, 1000 AE, Netherlands

Abstract:Rotational spectra of four isotopically enriched, singly substituted species of acrylonitrile have been studied up to 1.2 THz. Extensive analysis of the spectra recorded for H₂13CCHCN, H₂CCH¹³CN, H₂CCHC¹⁵N, and H₂CCDCN, revealed the presence of the same characteristic perturbations between the ground state and the $v_{11} = 1$ excited vibrational state, that have recently been identified in the parent molecule. For this reason transitions in $v_{11} = 1$ have also been assigned in each of the four isotopic species and a coupled state analysis of g.s. and $v_{11} = 1$ was performed on a total of around 3000 lines for each species. The derived precise values of $E(v_{11} = 1)$ are found to be consistent with estimates from anharmonic force field calculations. In addition, transitions for six new doubly substituted isotopic species of acrylonitrile, H₂13C¹³CHCN, H₂13CCH¹³CN, H²2C¹³CH¹³CN, H₂13CCHC¹⁵N, H₂C¹³CHC¹⁵N, and H²2CCH¹³C¹⁵N, have been assigned, and their ground state spectroscopic constants have been determined. Rotational constants for all known isotopic species of acrylonitrile have been combined with ab initio calculation of vibration-rotation constants in the first evaluation of the reSE geometry of this molecule.

Number of references:30