

148

Accession number:20123915459778

Title:Terahertz and far-infrared synchrotron spectroscopy and global modeling of methyl mercaptan, CH₃SH

Authors:Xu, Li-Hong (1); Lees, R.M. (1); Crabbe, G.T. (1); Myshrall, J.A. (1); Müller, H.S.P. (2); Endres, C.P. (2); Baum, O. (2); Lewen, F. (2); Schlemmer, S. (2); Menten, K.M. (3); Billingham, B.E. (4)

Author affiliation:(1) Centre for Laser, Atomic and Molecular Physics (CLAMS), Department of Physics, University of New Brunswick, 100 Tucker Park Road, Saint John, NB E2L 4L5, Canada; (2) I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany; (3) Max-Planck-Institut für Radioastronomie, 53121 Bonn, Germany; (4) Canadian Light Source Inc., University of Saskatchewan, 101 Perimeter Road, Saskatoon, SK S7N 0X4, Canada
Corresponding author:Xu, L.-H.(lxu@unb.ca)

Source title:Journal of Chemical Physics

Abbreviated source title:J Chem Phys

Volume:137

Issue:10

Issue date:September 14, 2012

Publication year:2012

Article number:104313

Language:English

ISSN:00219606

CODEN:JCPSA6

Document type:Journal article (JA)

Publisher:American Institute of Physics, 2 Huntington Quadrangle, Suite N101, Melville, NY 11747-4502, United States

Abstract:In this work, terahertz and Fourier transform far-infrared (FTFIR) synchrotron spectra of methyl mercaptan, CH₃SH, have been investigated in order to provide new laboratory information for enhanced observations of this species in interstellar molecular clouds and star-forming regions. Like its methanol cousin, methyl mercaptan has particularly rich spectra associated with its large-amplitude internal rotation that extend throughout the THz and FIR regions. We have recorded new spectra for CH₃SH from 1.1-1.5 and 1.790-1.808 THz at the University of Cologne as well as high-resolution FTFIR synchrotron spectra from 50-550 cm⁻¹ at 0.001 cm⁻¹ resolution on the far-IR beam-line at the Canadian Light Source. Assignments are reported for rotational quantum numbers up to J = 40 and K = 15, and torsional states up to v₂ for the THz measurements and v₃ for the FTFIR observations. The THz and FTFIR measurements together with literature results have been combined in a global analysis of a dataset comprising a total of 1725 microwave and THz frequencies together with ~18000 FTFIR transitions, ranging up to v₂ and J_{max} = 30 for MWT_{Hz} and 40 for FTFIR. The global fit employs 78 torsion-rotation parameters and has achieved a weighted standard deviation of ~1.1. A prediction list (v₂, J ≤ 45 and K ≤ 20) has been generated from the model giving essentially complete coverage of observable CH₃SH transitions within the bandwidths of major new astronomical facilities such as HIFI (Heterodyne Instrument for the Far Infrared) on the Herschel Space Observatory,

ALMA (Atacama Large Millimeter Array), SOFIA (Stratospheric Observatory For Infrared Astronomy) and APEX (Atacama Pathfinder Experiment) to close to spectroscopic accuracy. © 2012 American Institute of Physics.

Number of references:33

Main heading:Terahertz spectroscopy

Controlled terms:Astronomy - Laboratories - Light sources - Methanol - Observatories - Quantum theory

Uncontrolled terms:Atacama large millimeter arrays - Atacama pathfinder experiments - Data sets - Far-infrared - Global analysis - Global modeling - Herschel space observatories - Heterodyne instruments - High resolution - Internal rotations - Interstellar molecular clouds - Methyl mercaptans - Rotational quantum numbers - Standard deviation - Star-forming region - Stratospheric observatory for infrared astronomies - Synchrotron spectra - Tera Hertz - THz frequencies - THz measurements - Torsional state

Classification code:931.1 Mechanics - 804.1 Organic Compounds - 801 Chemistry - 931.4 Quantum Theory; Quantum Mechanics - 744 Lasers - 657 Space Physics - 443 Meteorology - 657.2 Extraterrestrial Physics and Stellar Phenomena

DOI:10.1063/1.4745792

Database:Compendex

Compilation and indexing terms, Copyright 2012 Elsevier Inc.