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Title:Terahertz and far-infrared synchrotron spectroscopy and global modeling of methyl mercaptan, $CH_3{}^{32}SH$
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Abstract:In this work, terahertz and Fourier transform far-infrared (FTFIR) synchrotron spectra of methyl mercaptan, $CH_3SH$, 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 $CH_3SH$ 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 $cm^{-1}$ 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 $v_t$ = 2 for the THz measurements and $v_t$ = 3 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 $v_t$ = 2 and $J_{max}$ = 30 for MW/THz 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 ($v_t$=2, J=45 and K=20) has been generated from the model giving essentially complete coverage of observable $CH_3{}^{32}SH$ 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.
Number of references:33
Inspec controlled terms:Fourier transform spectra - infrared spectra - librational states - organic

compounds - rotational isomerism - rotational states - terahertz wave spectra

Uncontrolled terms:transition coverage - torsion-rotation parameters - global fit - Fourier transform far-infrared transitions - terahertz frequency - microwave frequency - global dataset analysis - FTIR - Fourier transform far-infrared measurements - terahertz measurements - torsional states - rotational quantum numbers - far-infrared beam-line - high-resolution Fourier transform far-infrared synchrotron spectra - far-infrared region - terahertz region - large-amplitude internal rotation - star-forming regions - interstellar molecular clouds - terahertz spectra - methyl mercaptan - global modeling - far-infrared synchrotron spectroscopy - terahertz spectroscopy - frequency 1.1 THz to 1.5 THz - frequency 1.79 THz to 1.808 THz - wave number 50 $cm^{-1}$ to 550 $cm^{-1}$

Inspec classification codes:A3320B Radiofrequency and microwave molecular spectra - A3310E Rotational analysis (molecular spectra) - A3310G Vibrational analysis (molecular spectra) - A3520P Molecular rotation, vibration, and vibration-rotation constants - A3520J Molecular barrier heights (internal rotation, inversion); rotational isomerism, conformational dynamics - A3320E Infrared molecular spectra

Numerical data indexing:frequency 1.1E+12 1.5E+12 Hz;frequency 1.79E+12 1.808E+12 Hz;wavelength 2.0E-04 1.818182E-05 m

Treatment:Theoretical or Mathematical (THR); Experimental (EXP)

Discipline:Physics (A)

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