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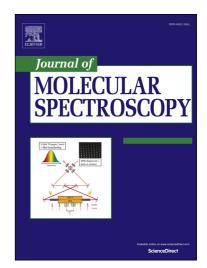
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ACCEPTED MANUSCRIPT

High resolution Fourier Transform Infrared Spectroscopy of the Ground State, ν_3 , $2\nu_3$ and ν_4 levels of $^{13}\text{CHF}_3$

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Abstract

We report high resolution ($\delta \tilde{\nu} \leq 0.001~\mathrm{cm}^{-1}$) Fourier Transform Infrared (FTIR) spectra of the trifluoromethane (fluoroform) isotopomer ¹³CHF₃ including results from synchrotron based spectroscopy at the Swiss light source (SLS). The analysis is extended to the pure rotational spectra in the Terahertz (farinfrared) range (15 to 100 cm⁻¹, $\delta \tilde{\nu}_{\rm FWHM} = 0.0006~\mathrm{cm}^{-1}$), the ν_3 fundamental ($\tilde{\nu}_0 = 695.2921~\mathrm{cm}^{-1}$) the associated "hot" band $2\nu_3 - \nu_3$ providing information on the level $2\nu_3$ ($\tilde{\nu}_0 = 1389.807~\mathrm{cm}^{-1}$) and the ν_4 fundamental ($\tilde{\nu}_0 = 1369.013~\mathrm{cm}^{-1}$) coupled to $2\nu_3$. The results are discussed in relation to the ¹³C isotope effect on the vibrational quantum dynamics as derived by theory and in relation to fluoroform as a greenhouse gas.

Keywords: $^{13}\text{CHF}_3$, fluoroform, high resolution infrared spectroscopy, FTIR, THz

1. Introduction

Fluoroform (trifluoromethane CHF₃, Figure 1) is a well known compound with a number of industrial uses and a resulting importance as a trace gas in the

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