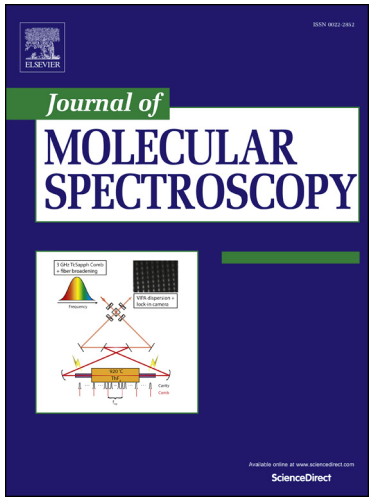

High resolution Fourier Transform Infrared Spectroscopy of the Ground State, $_3$,2_3 and $_4$ levels of $^{13}CHF_3$

I.B. Bolotova, O.N. Ulenikov, E.S. Bekhtereva, S. Albert, Z. Chen, H. Hollenstein, D. Zindel, M. Quack

PII: S0022-2852(17)30087-5
DOI: http://dx.doi.org/10.1016/j.jms.2017.05.003
Reference: YJMSP 10899

To appear in: *Journal of Molecular Spectroscopy*

Received Date: 15 February 2017
Revised Date: 5 May 2017
Accepted Date: 8 May 2017

Please cite this article as: I.B. Bolotova, O.N. Ulenikov, E.S. Bekhtereva, S. Albert, Z. Chen, H. Hollenstein, D. Zindel, M. Quack, High resolution Fourier Transform Infrared Spectroscopy of the Ground State, $_3$,2_3 and $_4$ levels of $^{13}CHF_3$, *Journal of Molecular Spectroscopy* (2017), doi: http://dx.doi.org/10.1016/j.jms.2017.05.003

High resolution Fourier Transform Infrared Spectroscopy of the Ground State, ν_3, $2\nu_3$ and ν_4 levels of $^{13}CHF_3$

I.B.Bolotova[a,b], O.N.Ulenikov[b,a], E.S.Bekhtereva[b,a], S.Albert[a], Z.Chen[a], H.Hollenstein[a], D.Zindel[a], M.Quack[a,*]

[a] *Physical Chemistry, ETH-Zürich, CH-8093, Zürich, Switzerland*
[b] *Institute of Physics and Technology, National Research Tomsk Polytechnic University, Tomsk 634050, Russia*

Abstract

We report high resolution ($\delta\tilde{\nu} \leq 0.001$ cm^{-1}) Fourier Transform Infrared (FTIR) spectra of the trifluoromethane (fluoroform) isotopomer $^{13}CHF_3$ including results from synchrotron based spectroscopy at the Swiss light source (SLS). The analysis is extended to the pure rotational spectra in the Terahertz (far-infrared) range (15 to 100 cm^{-1}, $\delta\tilde{\nu}_{\mathrm{FWHM}}$=0.0006 cm^{-1}), the ν_3 fundamental ($\tilde{\nu}_0$=695.2921 cm^{-1}) the associated "hot" band $2\nu_3-\nu_3$ providing information on the level $2\nu_3$ ($\tilde{\nu}_0$=1389.807 cm^{-1}) and the ν_4 fundamental ($\tilde{\nu}_0$=1369.013 cm^{-1}) coupled to $2\nu_3$. The results are discussed in relation to the ^{13}C isotope effect on the vibrational quantum dynamics as derived by theory and in relation to fluoroform as a greenhouse gas.

Keywords: $^{13}CHF_3$, fluoroform, high resolution infrared spectroscopy, FTIR, THz

1. Introduction

Fluoroform (trifluoromethane CHF_3, Figure 1) is a well known compound with a number of industrial uses and a resulting importance as a trace gas in the

*Corresponding author
Email address: martin@quack.ch (M.Quack)