COMPARISON OF ETHYLENE SPECTRA AT 10 μm RECORDED BY FOURIER TRANSFORM AND FREQUENCY COMB SPECTROMETERS

H. Ziadi[a,e], M. Rey[a], J. Tison[a], B. Grouiez[a], A. Voute[b], L. Manceron[c], V. Boudon[d], H. Aroui[e] and M. Rotger[a]

[a] Groupe de Spectrométrie Moléculaire et Atmosphérique , UMR CNRS 7331, Université de Reims Champagne-Ardenne, Moulin de la Housse B.P. 1039, F-51687 Reims Cedex 2, France
[b] AILES Beamline, Synchrotron SOLEIL, L'Orme des Merisiers, Départementale 128, 91190 Saint-Aubin, France
[c] Laboratoire Interuniversitaire des Systèmes Atmosphériques , Université Paris Cité, Université Paris-Est Créteil, CNRS, 75013 Paris, France
[d] Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 6303 CNRS - Université de Bourgogne, 9 Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France
[e]Laboratoire de Spectroscopie et de Dynamique Moléculaire (LSDM), École Nationale Supérieure d'Ingénieurs de Tunis, Université de Tunis, 5 Av Taha Hussein, 1008 Tunis, Tunisie

High-resolution Fourier transform infrared (FTIR) spectra of methyl fluoride (CH_3F) were recorded in the mid- and far-infrared regions using the Bruker IFS 125HR spectrometers at GSMA (Reims, France) and at the SOLEIL synchrotron facility (Saint-Aubin, France). The measurements cover both the pure rotational transitions of the ground state (20 – 100 cm^{-1}) and the vibrational triad region (1950 – 2450 cm^{-1}), which includes the $2\nu_3$, $\nu_3 + \nu_6$, and $2\nu_6$ bands. Spectra were recorded under various pressure conditions to optimize line visibility, with a high resolution. Line assignments were performed using predictions from the tensorial effective Hamiltonian implemented in the MIRS package, together with a newly developed automated assignment tool, SpectraMatcher, which facilitates line matching and discrimination of CH_3F transitions from overlapping CO_2 features. More than 5000 transitions (up to $J = 52$ in the ground state and up to $J = 45$ in the triad and $K = 19$) were assigned and included in a global fit. The sixth-order tensorial effective Hamiltonian model yielded excellent agreement with experiment, with root-mean-square (RMS) deviations better than 7×10^{-4} cm^{-1} across all regions. This paper presents the first continuous rovibrational study of CH_3F over both the triad and far-infrared ground state regions. The improved accuracy from previous studies stems from the improved set of effective Hamiltonian parameters which will also form a good basis from future applications in atmospheric modelling and spectroscopic databases.