

COMPOSITE ABSORPTION CROSS SECTIONS AND INTEGRATED BAND INTENSITIES OF CHF₃ IN SYNTHETIC AIR

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CHF₃ (fluoroform, trifluoromethane, HFC-23, CAS no: 75-46-7) is a strong potent greenhouse gas (GWP-100 = 14600), with its atmospheric amount fraction increasing by 0.75 ± 0.02 pmol/mol/year¹. It is not only a byproduct of the synthesis of CHClF₂ but is also used in the semiconductor industry and as a low-temperature refrigerant.

CHF₃ is an oblate symmetric top molecule (C_{3v} point group) with three totally symmetric vibrations (ν_1 , ν_2 , ν_3) and three doubly degenerate vibrations (ν_4 , ν_5 , ν_6). Its congested absorption spectra contain not only transitions from ground state and hot bands for main isotopologue (¹²CHF₃), but also information on ¹³CHF₃, which bands appear nearby. Absorption in the region of ν_2/ν_5 dyad occurs in the atmospheric transparency window and is used for remote sensing.

In the current work, we recorded several spectra with different compositions of CHF₃ mixtures with synthetic air to reconstruct the cumulative spectrum at 296 K in the region of 550–2000 cm⁻¹. A similar algorithm was used in our work with CF₄ and SF₆ and in the PNNL database². CHF₃ turned out to be a more challenging molecule since the contribution of the self-broadening becomes visible already at absorber dilution ratios exceeding 1%. This can lead to distortion (broadening) of the cumulative absorption cross sections compared to those corresponding to strongly diluted samples. Nevertheless, adding concentrated samples to the average does not affect the integrated intensities.

We report on the integrated intensities in the region of the ν_3 , ν_2/ν_5 and ν_4 fundamental bands together with the overtone band of ν_6 and two combinations that involve ν_2 band, namely $\nu_2 + \nu_6$ and $\nu_2 + \nu_3$. The expanded uncertainties ($k = 2$) are below 1.8% for the reported fundamental bands.

The measurements and analysis were performed within the frame of the EMPIR project "Metrology for Climate Relevant Volatile Organic Compounds" (MetClimVOC)³. The spectra were recorded using a Bruker-125 HR spectrometer at the PTB EUMETRICSPEC infrastructure⁴.

¹[10.1016/j.jqsrt.2019.06.019](https://doi.org/10.1016/j.jqsrt.2019.06.019), A. M. Fernando, P. F. Bernath, C. D. Boone, *JQSRT*, **238**, 106540 (2019).

²[10.1366/0003702042641281](https://doi.org/10.1366/0003702042641281), S.W. Sharpe et al., *App. Spectrosc.*, **58**(12), 1452–1461 (2004).

³EMPIR project "Metrology for climate relevant volatile organic compounds", ([MetClimVOC](#)).

⁴Spectral reference data for atmospheric monitoring, ([EUMETRISPEC](#)).