

**COMPOSITE SPECTRUM OF CF<sub>4</sub> IN MIXTURES WITH AIR:  
INTENSITIES OF THE FUNDAMENTAL AND COMBINATION BANDS  
WITH COMPATIBLE UNCERTAINTIES.**

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Tetrafluoromethane (CF<sub>4</sub>) is a minor constituent of the atmosphere with high global warming potential. Its origin is mainly anthropogenic and related to aluminum refining and semiconductor manufacturing. The analysis of the highly congested infrared spectrum of CF<sub>4</sub> is notoriously difficult and involving millions of lines. Besides, hot-band transitions contribute significantly to the infrared intensities.<sup>1,2</sup>

In the current work, we recorded IR spectra of CF<sub>4</sub> in the mixtures with binary air at 296 K in the region 550-2000 cm<sup>-1</sup>. Using a commercial critical orifice gas mixer, complemented with conventional manometric mixing methods, allowed us to create the composite absorption cross-sections for mixtures at 500 mbar and 1000 mbar using a similar algorithm as in PNNL database<sup>3</sup>. Extensive uncertainty evaluation for every wavenumber was performed. The resulting spectra are free from the saturation effects and have comparable uncertainties over several orders of magnitude.

We evaluated the integrated intensities in the region of the  $\nu_4$ , and  $\nu_3$  fundamental bands and four binary combinations  $\nu_2 + \nu_4$ ,  $\nu_1 + \nu_4$ ,  $\nu_2 + \nu_3$  and  $\nu_3 + \nu_4$ . Expanded uncertainties (k=2) are below 1.3% for the fundamental band and 2.9% for the combination bands, with the main contribution coming from the uncertainty of absorption pathlength. An estimate of the IR forbidden  $\nu_1$  band was also possible. Comparison with available literature data as well as the values from TheoReTS Information System [2] result is presented.

The measurements and analysis were performed within the frame of the EMPIR project "Metrology for Climate Relevant Volatile Organic Compounds" (MetClimVOC)<sup>4</sup>. The spectra were recorded using a Bruker-125 HR spectrometer at the PTB EUMETRICSPEC infrastructure.<sup>5</sup>

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<sup>1</sup>10.1016/j.jqsrt.2017.06.039, M. Carlos et al., *JQSRT*, **201**, 75–93 (2017).

<sup>2</sup>10.1039/c8cp03252a, M. Rey et al., *PCCP*, **20**, 21008–21033 (2018).

<sup>3</sup>10.1366/0003702042641281, S.W. Sharpe et al., *App. Spectrosc.*, **58**(12), 1452–1461 (2004).

<sup>4</sup>EMPIR project "Metrology for climate relevant volatile organic compounds", (MetClimVOC).

<sup>5</sup>Spectral reference data for atmospheric monitoring, (EUMETRISPEC).