INTENSITIES IN THE COMPOSITE SPECTRUM OF SF_6 IN MIXTURES WITH AIR AT 296 K

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Sulfur hexafluoride (SF_6) is used and emitted in a variety of industrial processes, such as magnesium and aluminium production. Becoming a minor part of the atmosphere, however small, its amount and evolution are of interest because of the the globar warming potential of the molecule. Hence the studies of the infrared spectra, which can be used for remote sensing, are of importance. SF_6 is a spherical molecule with Oh symmetry group. High symmetry results in a complicated absorption features with many vibrational bands overlapping. A recent work[1] reports an increased contribution of the hot transitions.

In the current work, we recorded IR spectra of SF_6 in the mixtures of different compositions with binary air at 300 and 1000 mbar and 296 K in the region 550-2000 cm^{-1}. In the case of SF_6, an assumption that the contribution of self-shifting and self-broadening does not have a significant impact on the absorption profile was met. It was possible then to combine the spectra with different partial pressures but the same total pressure as the composite spectrum. A similar algorithm is used in the PNNL database[2].

Using the composite spectra, we evaluated the integrated intensities in the region of the ν_4, and ν_3 fundamental bands as well as four binary combinations $\nu_1 + \nu_3$, $\nu_1 + \nu_4$, $\nu_2 + \nu_3$ and $\nu_2 + \nu_4$. The extended uncertainties are below 1.2for the fundamental bands and 2.4% for the combinations, with the exception of the weakest $\nu_1 + \nu_4$ band, which has an uncertainty of 7.6%. Comparison with available literature data as well as the values from TheoReTS Information System [3] is presented.

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

[1] 10.1039/d0cp05727d, M. Rey et al., *PCCP*, **20**, 12115 (2021).
[2] 10.1366/0003702042641281, S.W. Sharpe et al., *App. Spectrosc.*, **58**(12), 1452–1461 (2004).
[3] 10.1016/j.jms.2016.04.006, M. Rey et al., *J. Mol. Spectrosc.*, **20**, 138–158 (2016).
[4] EMPIR project "Metrology for climate relevant volatile organic compounds", (MetClimVOC).
[5] Spectral reference data for atmospheric monitoring, (EUMETRISPEC).

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