



Synchrotron radiation and long path cryogenic cells: New tools and results for modelling SF₆ absorption in the 10 μm atmospheric window

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Sulfur hexafluoride (SF₆) is a heavy and stable molecule used in many sectors, such as the electrical industry, but also as a gas tracer to model air mass motions in the Earth atmosphere. This anthropogenic species is also an atmospheric pollutant owing to its greenhouse effect capability. Although its six fundamental modes have been largely studied up to now, it is not the case for the numerous hot bands that represent the most important part of the SF₆ spectrum at room temperature. So, to model correctly the SF₆ atmospheric absorption requires the knowledge of the spectroscopic parameters of all states involved in these hot bands. Nevertheless, due to their overlapping, a direct analysis of the hot bands near the 10.5 μm absorption of SF₆ in the atmospheric window is not possible. It is necessary to use another strategy, gathering information in the far and mid infrared regions on initial and final states to recompute the relevant total absorption.

Here, we present new results of an analysis of spectra recorded at the AILES beam line at the SOLEIL Synchrotron facility. For these measurements, we used a IFS125HR interferometer in the 100 - 3200 cm⁻¹ range, coupled to a cryogenic multiple pass cell [1]. The optical path length was adjusted to 93m; the SF₆ sample was cooled down to 153 K. We could record 17 rovibrational bands of SF₆ in this region with a resolution of 0.0025 cm⁻¹. These results allowed us to perform the detailed analysis of several bands. Adding to previous knowledge on ν_3 , ν_2 , $2\nu_3$ and new results on $3\nu_3$, $2\nu_1 + \nu_3$, $\nu_1 + \nu_3$, $\nu_2 + \nu_3$, $\nu_3 - \nu_2$, $\nu_3 - \nu_1$, we developed a global fit of the ν_1 , ν_2 , ν_3 parameters, thus permitting the modelling of the $\nu_3 + \nu_1 - \nu_1$, $\nu_3 + \nu_2 - \nu_2$ hot bands. New information has also been obtained on ν_6 and $\nu_3 + \nu_5$ and another strategy will be detailed to model the more important $\nu_3 + \nu_5 - \nu_5$ and $\nu_3 + \nu_6 - \nu_6$ hot band contributions. Including these new parameters in the XTDS model [2], we substantially improved the previous global fit [3] of SF₆ parameters.

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[2] C. Wenger, V. Boudon, M. Rotger, M. Sanzharov, and J.-P. Champion, "XTDS and SPVIEW: Graphical tools for Analysis and Simulation of High Resolution Molecular Spectra", J. Mol. Spectrosc. 251, 102 (2008).

[3] M. Faye, A. Le Ven, V. Boudon, L. Manceron, P. Asselin, P. Soulard, F. Kwabia Tchana, P. Roy, *High-Resolution spectroscopy of difference and combination bands of SF₆ to elucidate the $\nu_3 + \nu_1 - \nu_1$ and $\nu_3 + \nu_2 - \nu_2$ hot band structures in the ν_3 region*, Mol. Phys. 112, 909059 (2014).