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(I) Radiative efficiency and global warming potential of fluorinated greenhouse gases

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The phase-out of ozone depleting substances has led to the release in the atmosphere of new generations of fluorinated coolants and propellants. Those molecules contain C-F bonds, which make them strong absorbers in the mid-infrared spectral region. To properly assess the impact of those molecules on climate, their radiative forcing must be calculated from their experimental and/or theoretical absorption cross-sections.
The common way to obtain the data is through the acquisition of laboratory absorption spectra by Fourier transform spectroscopy. This process allows the study of the temperature and pressure dependence as well as the impact of hot bands and combination bands. However, the acquisition is time-consuming and not always straightforward.
A second method consists into calculating the vibrational band positions and intensities of the molecule by quantum mechanical calculations and simulating the cross-section spectra. The calculations can be carried out by ab-initio or density functional theory methods. Although theoretical data can quickly estimate the radiative efficiency of a molecule, the results are dependent on the levels of theory and still require empirical corrections to match their experimental counterparts. However, theoretical calculations has proven to be an efficient tool to analyze the conformational populations and to provide data on a spectral range that cannot be easily accessed experimentally.
Over the past few years, our group has analyzed the radiative properties of multiple molecules and extracted their radiative efficiency and global warming potential. In this talk, we will discuss recent results and findings. In particular, we will show that the best results come from a compilation of both experimental and theoretical results.

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