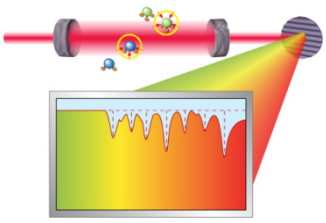
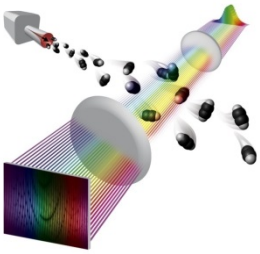
Optical Frequency Comb Spectroscopy Group announces thesis work:

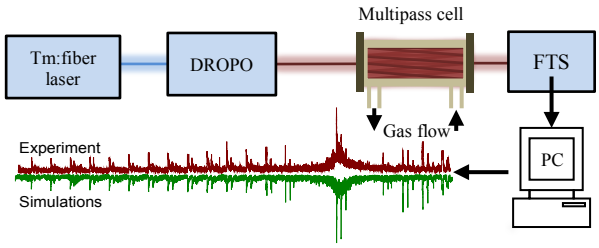
Simulations of broadband high-resolution spectra of complex atmospheric molecules



Our group works with the development and applications of ***optical frequency comb spectroscopy*** for broadband ultrasensitive detection of molecular species in gas phase. Optical frequency combs are produced by femtosecond mode-locked lasers, whose spectrum consists of a comb of narrow laser lines covering a very broad spectral range. Spectroscopy performed with optical frequency combs is equivalent to a measurement with thousands of synchronized laser lines and allows highly sensitive simultaneous detection of many molecular species in short acquisition times. Therefore the technique has the potential to become the ultimate tool for trace gas detection for environmental monitoring, industrial process control or medical diagnostics.



Monitoring key ***atmospheric species*** such as halogen-containing compounds is essential because of their significant influence on the lifetimes and the budget of many climatically active gases. We are using mid-infrared optical frequency comb spectroscopy to measure — for the first time — broadband high-resolution absorption spectra of brominated and chlorinated methanes. Our system is based on a synchronously pumped (pump source: Tm:fiber laser) doubly-resonant optical parametric oscillator (DROPO), a multipass cell, and a Fourier transform spectrometer (FTS). To retrieve the information about the composition and concentration of the sample from its absorption spectrum, a theoretical model of the spectrum must be fitted to the experimental data. However, such theoretical models do not exist for the targeted molecules. These models can be developed by ***simulating high-resolution spectra*** and fitting them to highly accurate experimental spectra of known sample composition and concentration. The spectral simulations can be carried out with the help of already existing simulation packages (e.g., PGOPHER software: a user friendly spectral simulation routine developed by a research team at Bristol University). The output fit parameters, e.g., line positions and line strengths, will be used to develop models for unknown sample concentrations.



The ***aim of this project*** is to simulate a theoretical model of high-resolution spectrum of bromoform ($CHBr_3$) and verify it using the experimental data measured using our spectrometer. Within this thesis project you will get hands-on experience with advanced spectroscopic techniques and learn to use spectral simulation tools. The project is suitable for a student with interest in ***spectral simulations and molecular spectroscopy***.

If you wish to obtain more information about the project and visit our lab please contact Aleksandra Foltynowicz (aleksandra.foltynowicz@umu.se).