

Exercise No. 2 – Vibration

You can reuse the controlfiles from the first exercise to answer the questions on vibrational spectra. First, copy the controlfile into this directory:

```
$ cd ~/arts-lectures/exercises/02-vibrational_spectra/  
$ cp ../01-rotational_spectra/absorption.arts vibration.arts
```

Next, you have to adjust the controlfile to perform simulations at higher frequencies. The catalogue storing the information on line absorption used in the first exercise is limited to frequencies below 3 THz. You have to replace it with `HiTranSplit/`, which covers a wider range of frequencies. The frequency range has to be extended when reading the line catalogue (`abs_linesReadFromSplitArtscat`) and when setting the frequency grid (`f_grid`) for the simulation.

Afterwards, you can create a directory for the results and start the ARTS simulation:

```
$ mkdir results  
$ arts vibration.arts
```

Plot the calculated absorption cross sections as a function of wavenumber. For this purpose, you can copy and adapt the plotting script from the exercise on rotational bands. Remember to create a `plots/` directory before running the scripts.

1. Find the fundamental band of CO and plot its spectrum.
 - Determine the band center frequency $\hat{\nu}$ from your plot.
 - There is some “pollution” in the P-branch that comes from lines of ^{13}CO . Recalculate the spectrum for only the main isotopologue.
2. Explore the spectrum of either H_2O or CO_2 . Can you find the different vibration bands?