

Exercise 2: Vibrational spectra

Sample Solution

Effective: 25.11.2016

1. Find the fundamental band of CO and plot its spectrum.
 - Determine the band center frequency $\tilde{\nu}$ from your plot. Figure 1 shows the absorption band of CO .
 - The center frequency is around $\tilde{\nu} = 2143\text{ cm}^{-1} = 64.2\text{ GHz}$.
 - There is some “pollution” in the P-branch that comes from lines of ^{13}CO . Recalculate the spectrum for only the main isotopologue.
 - The recalculated spectra for the main isotopologue is shown in Figure 2.

2. Explore the spectrum of either H_2O or CO_2 . Can you find the different vibration bands?

Figure 3 shows the absorption bands of both, CO_2 and H_2O . Those two gases are the main causer of the green house effect. It shows that both gases are absorbing in different spectral regions.

The symmetric stretch mode of CO_2 at 1330 cm^{-1} is not associated with a change in the dipole moment, and therefore is not infrared active. The visible weak bands away from the fundamental frequencies could be:

- hot bands
- isotopologue bands
- ...

You could easily verify the first two alternatives by explicitly selecting only one isotope, or by recalculating with a very high or very low temperature.

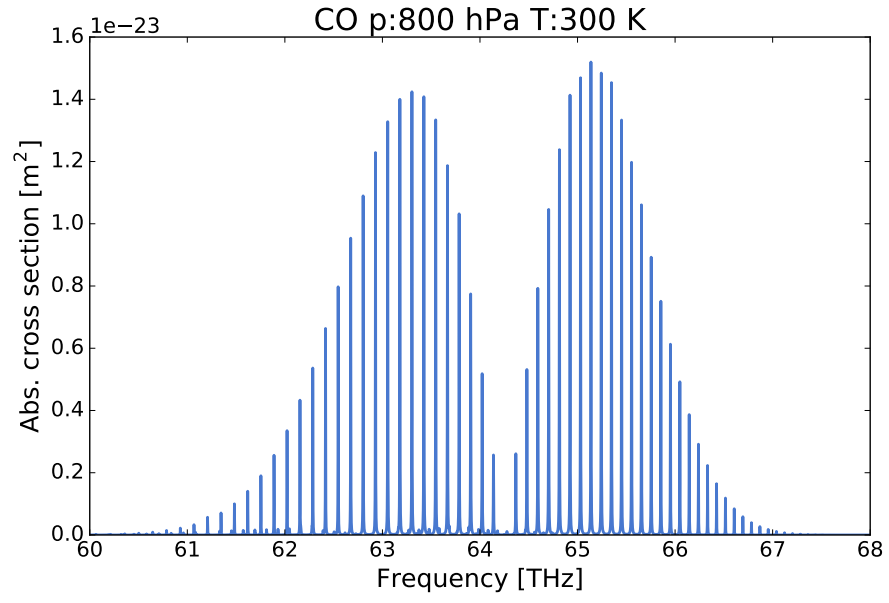


Figure 1: Absorption cross section for CO (all stable isotopologues).

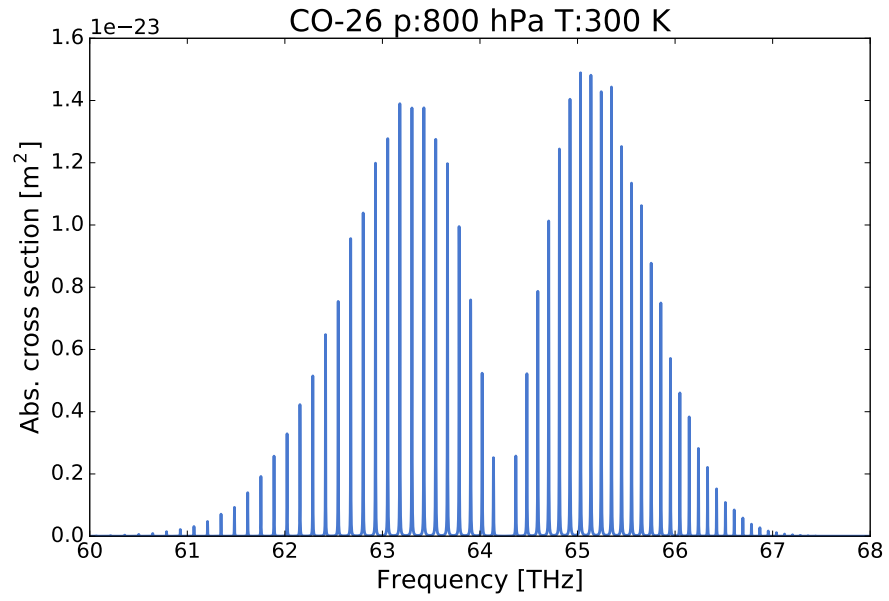


Figure 2: Absorption cross section for CO (main isotopologue).

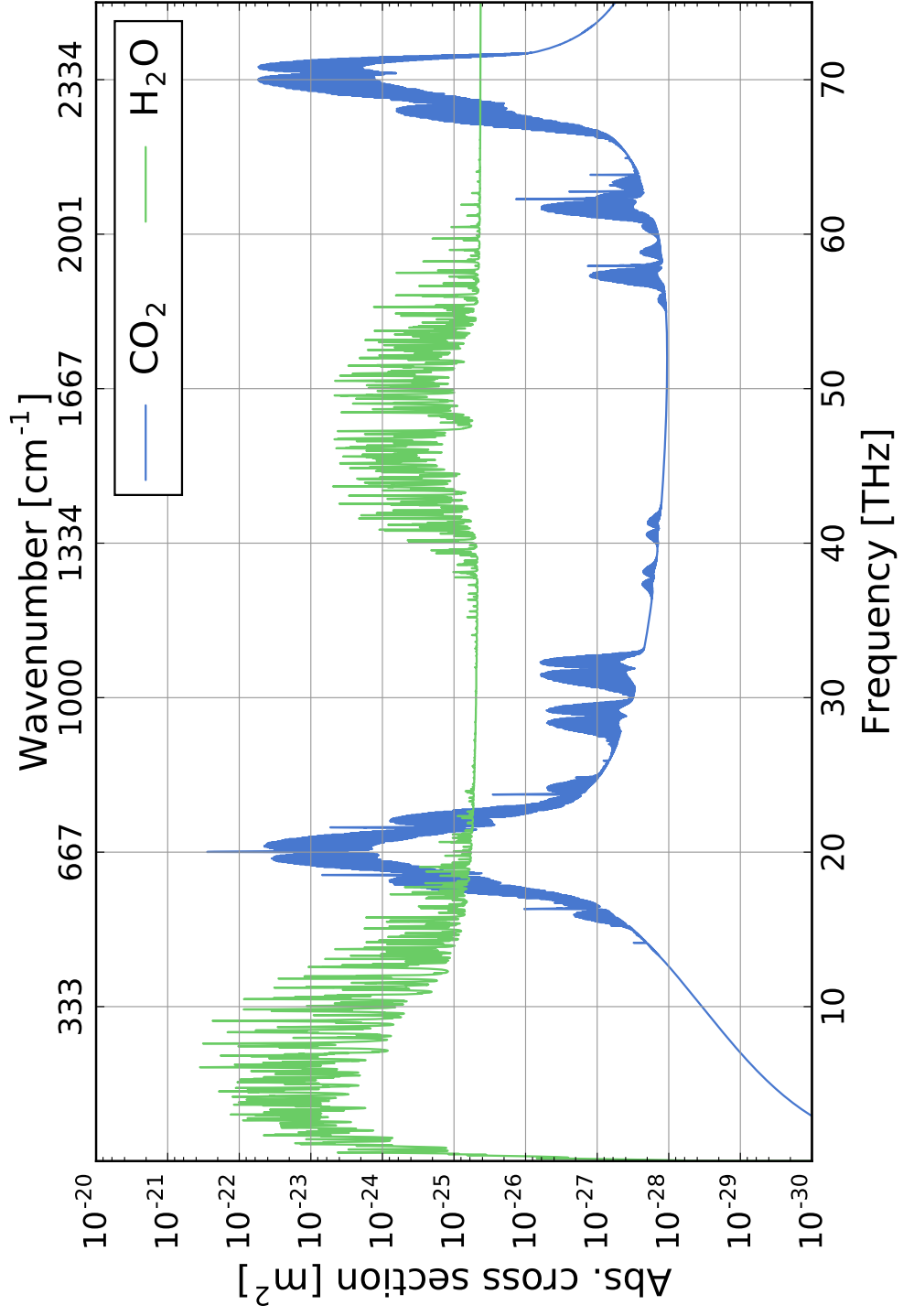


Figure 3: Absorption cross sections for CO_2 and H_2O .