

# 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  $1330\text{ cm}^{-1}$  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 are isotopologue bands; the isotopologue is no longer symmetric and the fundamental becomes visible.

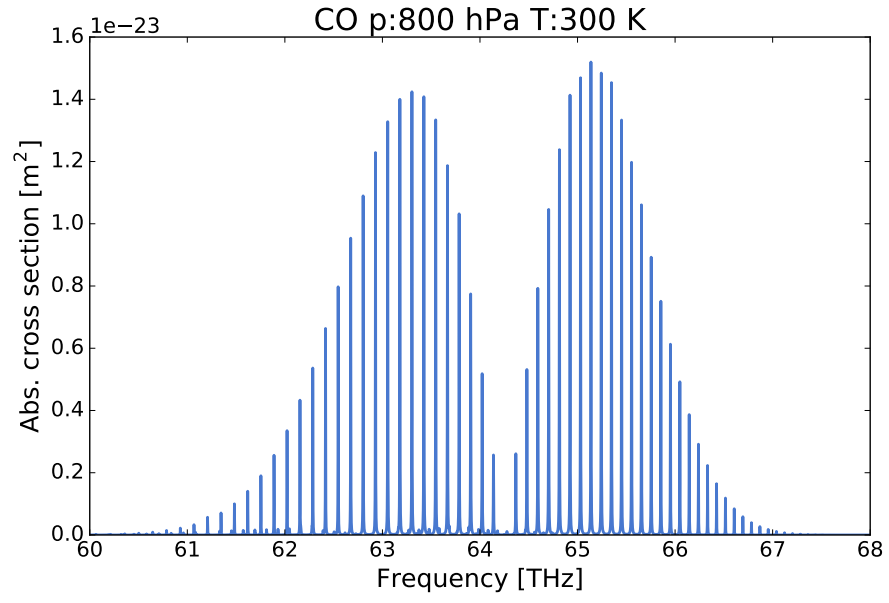


Figure 1: Absorption cross section for *CO* (all stable isotopologues).

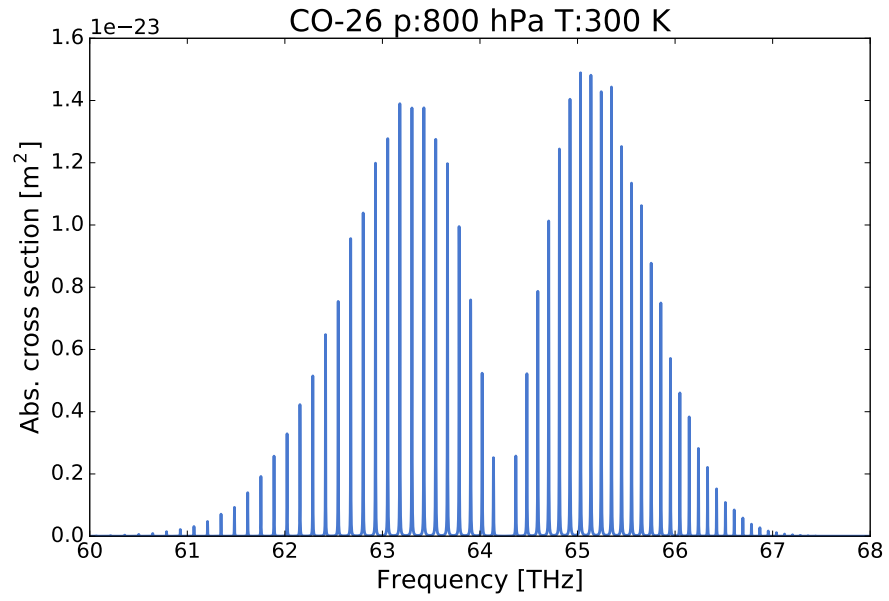


Figure 2: Absorption cross section for *CO* (main isotopologue).

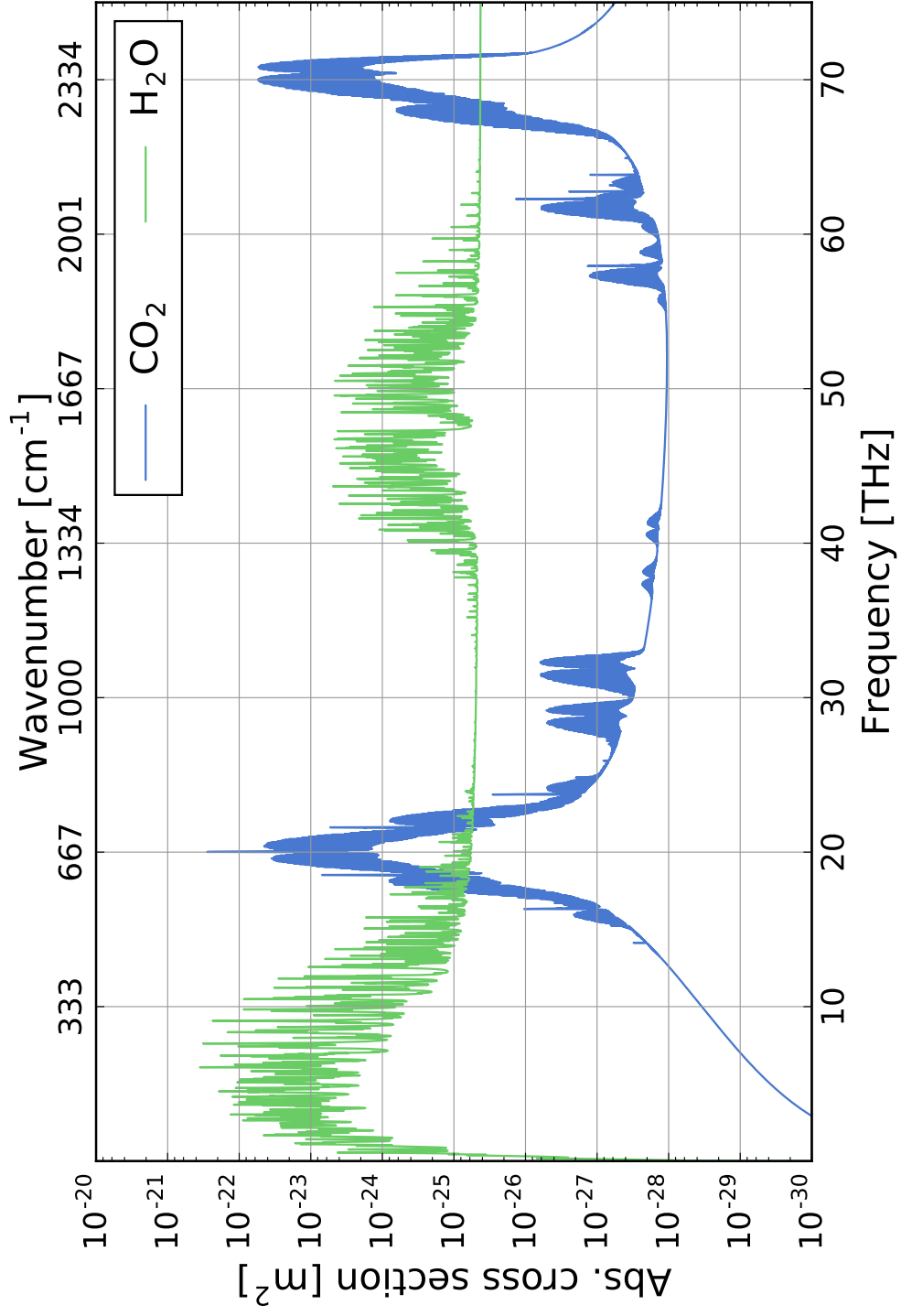


Figure 3: Absorption cross sections for  $\text{CO}_2$  and  $\text{H}_2\text{O}$ .