ASTR/ATOC 5560 Problem Solving Solutions Week 4

1. Between 691 cm⁻¹ and 693 cm⁻¹ the HITRAN 2000 database contains the following parameters for lines of the relevant gases with line strengths above 10^{-21} cm/molecule:

31	691.370100	1.040E-21	8.869E-04.0761.1003	228.7342	.76
21	691.972498	9.167E-20	9.167E-03.0684.0869	362.7882	.78
31	692.034800	1.160E-21	9.060E-04.0767.1009	191.7092	.76
21	692.129032	4.010E-21	9.500E-03.0686.0878	1007.1335	.78
21	692.400132	3.685E-21	9.484E-03.0684.0869	1031.1291	.78
31	692.468700	1.240E-21	9.110E-04.0771.1016	158.1653	.76
31	692.661600	1.070E-21	7.898E-04.0780.1038	78.5386	.76
31	692.696400	1.240E-21	8.823E-04.0775.1023	128.1196	.76
31	692.748400	1.190E-21	8.469E-04.0778.1030	101.5791	.76

We would like to compute the optical depth at a wavenumber of 692.000 cm⁻¹ for a 1 km thick layer at a pressure of p = 102 mb and temperature of T = 217 K. The volume mixing ratios of the radiatively active gases are $q_{H2O} = 6.55 \times 10^{-6}$, $q_{CO2} = 3.70 \times 10^{-4}$, and $q_{O3} = 2.22 \times 10^{-6}$. The number of air molecules per cm² in this layer is

$$u_{air} = \frac{\Delta z N_A p}{R^* T} = 3.40 \times 10^{23} \text{ molec/cm}^2$$
.

a) Determine the single absorption line that will dominate the absorption at 692.000 cm⁻¹. Write down the molecule and wavenumber.

The important absorption line is the one at 691.9725 cm⁻¹ which is from the main isotope of CO₂. The other CO₂ lines have lower strengths and are much further in terms of line halfwidths from 692 cm⁻¹. The nearby ozone line is not relevant since the ozone abundance is 167 times less than CO₂ and the line strength at 296 K is about 80 times less.

b) Calculate the Lorentz halfwidth for this absorption line. Self-broadening can be ignored since the mixing ratios are so small.

The halfwidth of the Lorentz line shape scales according to

$$\alpha = \alpha_0 \left(\frac{p}{p_0}\right) \left(\frac{T_0}{T}\right)^n$$

where α_0 is the halfwidth in the HITRAN database at pressure $p_0 = 1013.25$ mb and temperature $T_0 = 296$ K. The halfwidth of this line is

$$\alpha = (.0684 \text{ cm}^{-1}) \left(\frac{102 \text{ mb}}{1013 \text{ mb}}\right) \left(\frac{296 \text{ K}}{217 \text{ K}}\right)^{0.78} = 0.00877 \text{ cm}^{-1}$$

c) Calculate the line stength for this absorption line at the temperature of this layer. The partition functions are

Molecule/Isotope	Q(217 K)	Q(296 K)
21	198.4	286.2
31	2094.4	3481.9

The line strength scales as

$$S_i(T) = S_i(T_0) \frac{\exp(-hcE_{L,i}/k_B T)Q_T(T_0) \left[1 - \exp(-hc\nu_{0,i}/k_B T)\right]}{\exp(-hcE_{L,i}/k_B T_0)Q_T(T) \left[1 - \exp(-hc\nu_{0,i}/k_B T_0)\right]}$$

where T is the temperature, T_0 is the reference temperature (296 K), Q_T is the total partition function for the particular molecule/isotope, $E_{L,i}$ is the lower state energy in cm⁻¹, and $\nu_{0,i}$ is the transition wavenumber.

For this CO₂ absorption line the line strength is

$$S_{i}(T) = S_{i}(T_{0}) \frac{\exp\left[-\frac{(1.4388 \text{ K cm})(362.7882 \text{ cm}^{-1})}{217 \text{ K}}\right]}{\exp\left[-\frac{(1.4388 \text{ K cm})(362.7882 \text{ cm}^{-1})}{296 \text{ K}}\right]} \frac{286.2}{198.4} \frac{\left(1 - \exp\left[-\frac{(1.4388 \text{ K cm})(691.9725 \text{ cm}^{-1})}{217 \text{ K}}\right]\right)}{\left(1 - \exp\left[-\frac{(1.4388 \text{ K cm})(691.9725 \text{ cm}^{-1})}{296 \text{ K}}\right]\right)}$$
$$S_{i}(T) = (9.167 \times 10^{-20} \text{ cm/molec}) \left(\frac{0.090}{0.171}\right) (1.443) \left(\frac{0.9898}{0.9654}\right)$$
$$S_{i}(T) = (9.167 \times 10^{-20} \text{ cm/molec}) (0.526) (1.443) (1.025) = 7.136 \times 10^{-20} \text{ cm/molec}$$

d) Calculate the absorption coefficient and optical depth of this layer at 692 cm⁻¹.

Since we are considering a single Lorentz absorption line, we use the Lorentz line shape f. The the absorption coefficient is given by

$$k_{\nu} = Sf(\nu - \nu_0) = \frac{S\alpha/\pi}{(\nu - \nu_0)^2 + \alpha^2}$$

For the desired wavenumber of $\nu=692.000~{\rm cm^{-1}}$ the monochromatic absorption coefficient is

$$k_{\nu} = \frac{(7.136 \times 10^{-20} \text{ cm/molec})(0.00877 \text{ cm}^{-1})/\pi}{(692.0000 \text{ cm}^{-1} - 691.9725 \text{ cm}^{-1})^2 + (0.00877 \text{ cm}^{-1})^2} = 2.39 \times 10^{-19} \text{ cm}^2/\text{molec}$$

The optical depth of the layer at this wavenumber is the absorber amount of CO_2 times the absorption coefficient

$$\tau_n u = k_{\nu} u_{CO2} = k_{\nu} q_{CO2} u_{air}$$

$$\tau_n u = (2.39 \times 10^{-19} \text{ cm}^2/\text{molec})(3.70 \times 10^{-4})(3.40 \times 10^{23} \text{ molec}/\text{cm}^{-2}) = 30.1$$