

Chapter 6. Molecular Spectroscopy: Applications

Notes:

- *Most of the material presented in this chapter is adapted from Stahler and Palla (2004), Chap. 6, and Appendices B and C.*

6.1 Carbon Monoxide (CO)

Since molecular hydrogen H_2 does not possess an electric dipole moment, and is therefore impossible to detect in the most parts of molecular clouds where temperatures are too low to vibrationally excite it, it is imperative to use other molecules to probe the molecular content of the interstellar medium. The main species of carbon monoxide, $^{12}C^{16}O$, and some of its isotopologues (i.e., $^{13}C^{16}O$, $^{12}C^{18}O$, etc.) are most commonly used for this task. Carbon monoxide is a very stable molecule, with a triple-bond between the two nuclei, and highly abundant. It is, in fact, the second most abundant molecule in the interstellar medium with a relative abundance to H_2 of approximately 10^{-4} . Figure 6-1 shows examples of spectra from three carbon monoxide isotopologues in the $J = 2 \rightarrow 1$ rotational transition in DR21(OH), a well-known star-forming region. These data were obtained at the Caltech Submillimeter Observatory, located on Mauna Kea, Hawaii, in October 2007.

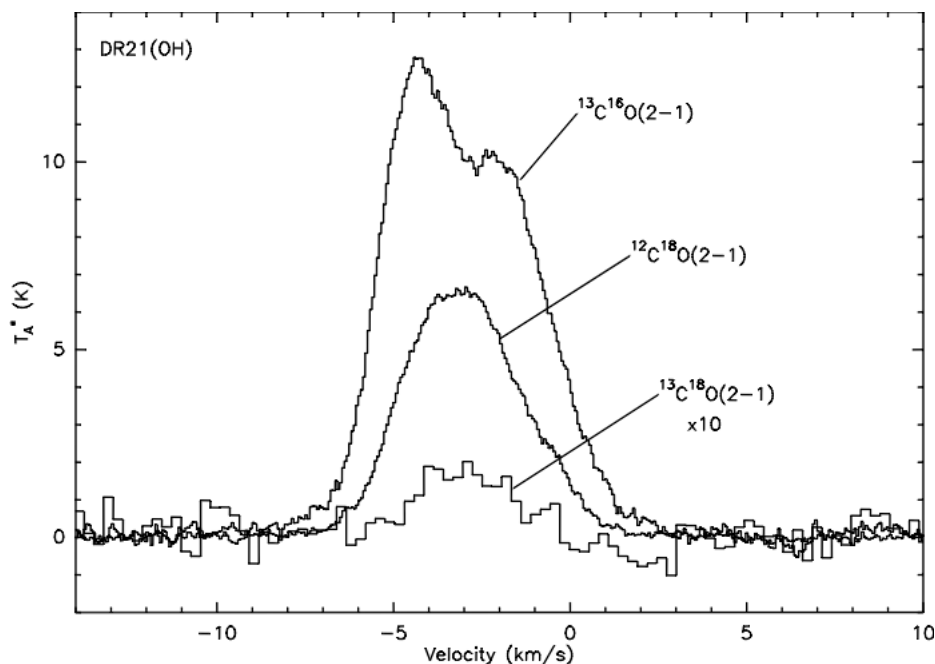


Figure 6-1 - Spectra of the $J = 2 \rightarrow 1$ rotational transition from the $^{13}C^{16}O$, $^{12}C^{18}O$, and $^{13}C^{18}O$ molecular species in the DR21(OH) star-forming region. Note that the $^{13}C^{18}O$ spectrum temperature is multiplied by a factor of ten (adapted from Hezareh et al. 2008, ApJ, 684, 1221).

6.1.1 The Detection Equation

We start by revisiting equation (2.25) we previously derived for the specific intensity I_ν measured at some location away from an emitting region, of source function S_ν , which is also located between the point of observation and some background emission $I_\nu(0)$. We have shown that

$$I_\nu = I_\nu(0)e^{-\tau_\nu} + S_\nu(1 - e^{-\tau_\nu}), \quad (6.1)$$

where τ_ν is the optical depth through the emitting region. We will now somewhat refine the treatment we presented in Section 3.1.1 and consider the difference $I_\nu - I_\nu(0)$, which we will equate to the intensity of a black body of (brightness) temperature T_B in the Rayleigh-Jeans limit

$$I_\nu - I_\nu(0) = \frac{2\nu^2}{c^2} kT_B. \quad (6.2)$$

The reason for considering $I_\nu - I_\nu(0)$ and not $I_\nu - I_\nu(0)e^{-\tau_\nu}$ is that usually during an observation the telescope will first be pointed on the source (commonly called *ON-position* or *ON-source*), where I_ν is measured, and then at a point away for the emitting region on the plane of the sky where only $I_\nu(0)$ is present (*OFF-position* or *OFF-source*); this method of observation is often referred to as **beam switching**. Combining equations (6.1) and (6.2) we have

$$I_\nu - I_\nu(0) = [S_\nu - I_\nu(0)](1 - e^{-\tau_\nu}), \quad (6.3)$$

or

$$T_B = \frac{c^2}{2k\nu^2} [S_\nu - I_\nu(0)](1 - e^{-\tau_\nu}). \quad (6.4)$$

Finally, we further assume that both the source and background intensities can be well approximated by Planck's blackbody functions of temperature T_{ex} and T_{bg} , respectively ('ex' stands for 'excitation'). We can therefore write the so-called **detection equation** as

$$T_B = T_0 \left(\frac{1}{e^{T_0/T_{\text{ex}}} - 1} - \frac{1}{e^{T_0/T_{\text{bg}}} - 1} \right) (1 - e^{-\tau_\nu}), \quad (6.5)$$

where $T_0 \equiv h\nu/k$ is the equivalent temperature of the transition responsible for the detected radiation.

6.1.2 Temperature and Optical Depth

Using the spectra of Figure 6-1 and the previously derived equations we determine some fundamental parameters characterizing the physical conditions pertaining to the DR21(OH) molecular cloud. These spectra for the detections of the $J = 2 \rightarrow 1$ rotational transition of the $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$, and $^{13}\text{C}^{18}\text{O}$ molecular species arise at frequencies of 220.4 GHz, 219.6 GHz, and 209.4 GHz, respectively. The telescope efficiency is $\eta \approx 0.65$ at these frequencies, and will be used to relate the antenna and brightness temperatures with $T_A^* = \eta T_B$ (see Section 3.1.1 of the Lecture Notes).

We first apply the detection equation (6.5) to the line centre of the $J = 2 \rightarrow 1$ transition of $^{13}\text{C}^{16}\text{O}$. We therefore respectively denote by τ_0 and ν_0 the optical depth and frequency at the line centre where $\nu_{\text{lsr}} \approx -3 \text{ km s}^{-1}$ (we use the same subscript for other quantities), and assign $T_{\text{bg}} = 2.7 \text{ K}$ for the background radiation temperature (i.e., we use the temperature of the cosmic microwave radiation or CMB). It is probably very reasonable to expect that this line is optically thick, i.e., $\tau_0(^{13}\text{C}^{16}\text{O}) \gg 1$ and from equation (6.5)

$$T_{\text{B}_0} \approx T_0 \left(\frac{1}{e^{T_0/T_{\text{ex}}} - 1} - \frac{1}{e^{T_0/T_{\text{bg}}} - 1} \right) \quad (6.6)$$

at the line centre. we also have

$$T_0 = \frac{h\nu_0}{k_B} = \frac{6.63 \times 10^{-27} \cdot 220.4 \times 10^9}{1.38 \times 10^{-16}} = 10.6 \text{ K}, \quad (6.7)$$

and from Figure 6-1

$$T_{\text{B}_0} \approx \frac{10 \text{ K}}{0.65} = 15.4 \text{ K}. \quad (6.8)$$

Inverting equation (6.6) for $T_{\text{ex}}(^{13}\text{C}^{16}\text{O})$ we find that

$$\begin{aligned} T_{\text{ex}}(^{13}\text{C}^{16}\text{O}) &= \frac{T_0}{\ln \left[1 + \left(\frac{T_{\text{B}_0}}{T_0} + \frac{1}{e^{T_0/T_{\text{bg}}} - 1} \right)^{-1} \right]} \\ &= 20.5 \text{ K}. \end{aligned} \quad (6.9)$$

Because this transition produces a line that is optically very thick, it is most likely that the corresponding population level is in **local thermodynamic equilibrium** (LTE). This is because radiation emanating from “far away” locations in the cloud cannot affect the gas locally. Furthermore, because T_0 is relatively low, i.e., on the order or less than the

expected gas temperature in a molecular cloud, the energy levels involved in this transition can easily be excited through collisions within the gas, and $T_{\text{ex}}(^{13}\text{C}^{16}\text{O})$ is therefore at a level that is perfectly suited for the kinetic temperature of the gas. We then write

$$T_{\text{ex}}(^{13}\text{C}^{16}\text{O}) = T_{\text{kin}}. \quad (6.10)$$

Although the corresponding $^{12}\text{C}^{18}\text{O}$ transition is not likely to be strongly optically thick, it is to be expected that this molecule will be coexistent with $^{13}\text{C}^{16}\text{O}$ and, therefore, subjected to similar physical conditions. Moreover, the $J = 2 \rightarrow 1$ transitions for these two molecular species have very similar characteristics (i.e., T_0 , n_{crit} , etc.). We therefore write that

$$T_{\text{ex}}(^{12}\text{C}^{18}\text{O}) = T_{\text{kin}} = 20.5 \text{ K}. \quad (6.11)$$

We calculate for this transition

$$T_0 = \frac{219.6}{220.4} \cdot 10.6 \text{ K} \approx 10.6 \text{ K}, \quad (6.12)$$

and from equation (6.5) we have

$$\begin{aligned} \tau_0(^{12}\text{C}^{18}\text{O}) &= -\ln \left[1 - \frac{T_{\text{B}_0}}{T_0} \left(\frac{1}{e^{T_0/T_{\text{ex}}} - 1} - \frac{1}{e^{T_0/T_{\text{bg}}} - 1} \right)^{-1} \right] \\ &= 1.0, \end{aligned} \quad (6.13)$$

where $T_{\text{B}_0} = 6.5 \text{ K}/0.65 = 10 \text{ K}$ was used. Since this transition is marginally optically thin or thick, we should be careful in assuming that isotopologues, such as $^{12}\text{C}^{18}\text{O}$, are unequivocally optically thin, as is too often asserted (see the comment from Stahler and Palla at the beginning of their Section 6.3.1).

On the other hand, considering the weakness of the $^{13}\text{C}^{18}\text{O}$ line, it is likely that the relation $\tau_0(^{13}\text{C}^{18}\text{O}) \ll 1$ is satisfied. We also assume that

$$T_{\text{ex}}(^{13}\text{C}^{18}\text{O}) = T_{\text{kin}} = 20.5 \text{ K}, \quad (6.14)$$

for the same reasons as in the case of $^{12}\text{C}^{18}\text{O}$ earlier and equation (6.5) then becomes

$$\tau_0 = \frac{T_{\text{B}_0}}{T_0} \left(\frac{1}{e^{T_0/T_{\text{ex}}} - 1} - \frac{1}{e^{T_0/T_{\text{bg}}} - 1} \right)^{-1}. \quad (6.15)$$

Using

$$T_0 = \frac{209.4}{220.4} \cdot 10.6 \text{ K} \approx 10.1 \text{ K}$$

$$T_{B_0} = \frac{0.18 \text{ K}}{0.65} \approx 0.28 \text{ K}$$
(6.16)

we have

$$\tau_0 \approx 0.02.$$
(6.17)

This value is much less than unity and, therefore, consistent with our assumption.

We note that the optical depth values obtained for these three transitions are qualitatively consistent with the appearances of their corresponding line profiles shown in Figure 6-1. More precisely, the $^{13}\text{C}^{16}\text{O}$ profile is heavily saturated (i.e., flattish) even showing signs of self-absorption (note the ‘dip’ near the line centre), both indications that its optical depth is much larger than unity; the $^{12}\text{C}^{18}\text{O}$ profile with $\tau_0(^{12}\text{C}^{18}\text{O}) \approx 1$ only shows the beginnings of saturation broadening; finally, although it is admittedly more difficult to judge in view of its weakness, the $^{13}\text{C}^{18}\text{O}$ line profile shows no obvious sign of saturation.

6.1.3 Transitions between Two Levels and Column Density

Let us now more generally consider a molecular species (e.g., $^{13}\text{C}^{18}\text{O}$ or any other molecule) that has a density n in a gas of total density n_{tot} . We want to study transitions between two levels separated by an energy difference $\Delta E = E_2 - E_1 > 0$ as a result of interaction due to radiation or collisions with other components of the gas; we denote by n_1 and n_2 the density of molecules in the lower and upper levels, respectively.

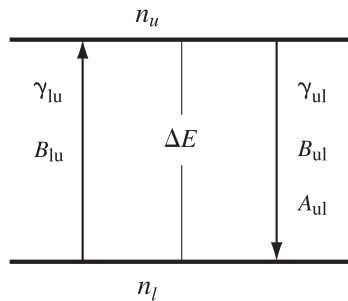


Figure 6-2 – Possible transitions between in a two-level system. Transitions due to collisions are represented by γ , while radiative transitions are represented by A and B .

Transitions due to collisions are represented by γ_{12} and γ_{21} , i.e., the total rate of collisional excitation per unit volume is given by $\gamma_{12}n_1n_{\text{tot}}$, etc. Transitions due to radiative processes are characterized by the **Einstein coefficients** B_{12} , B_{21} , and A_{21} . The rate of radiative excitation per unit volume from *absorption* is $B_{12}n_1\bar{J}$, the corresponding rate for the emission of photons from *stimulated emission* is $B_{21}n_2\bar{J}$, while the rate of *spontaneous emission* is $A_{21}n_2$. The quantity \bar{J} is related to the mean intensity (see eq. (2.19) in Chapter 2) through

$$\bar{J} = \int_0^\infty J_\nu \phi(\nu) d\nu, \quad (6.18)$$

with $\phi(\nu)$ the intrinsic line profile. This profile is centered at $\nu_0 = \Delta E/h$ and normalized with

$$\int_0^\infty \phi(\nu) d\nu = 1. \quad (6.19)$$

Under conditions of equilibrium the level populations will remain unchanged with time (in a statistical sense) and we have

$$\gamma_{12}n_1n_{\text{tot}} + B_{12}n_1\bar{J} = \gamma_{21}n_2n_{\text{tot}} + B_{21}n_2\bar{J} + A_{21}n_2. \quad (6.20)$$

For cases where collisions dominate ($\gamma n_{\text{tot}} \gg B\bar{J}$) we find that

$$\frac{\gamma_{12}}{\gamma_{21}} = \frac{n_2}{n_1}, \quad (6.21)$$

for which, under *local thermodynamic equilibrium* (LTE) conditions, the right-hand side must obey the Boltzmann distribution at the kinetic temperature T_{kin} that characterizes the collisions. That is,

$$\frac{\gamma_{12}}{\gamma_{21}} = \frac{g_2}{g_1} e^{-\Delta E/kT_{\text{kin}}}. \quad (6.22)$$

This equation will hold for any conditions.

On the other hand, when radiative processes completely dominate ($\gamma n_{\text{tot}} \ll B\bar{J}$) the system will come in equilibrium at the radiation temperature T_{rad} and equation (6.20) becomes

$$\bar{J} = \frac{A_{21}/B_{21}}{(g_1 B_{12}/g_2 B_{21}) e^{\Delta E/kT_{\text{kin}}} - 1}. \quad (6.23)$$

Since under equilibrium conditions the mean intensity must equal Planck's blackbody law, i.e., $J_\nu = B_\nu$, we have

$$\begin{aligned}\bar{J} &= \int_0^\infty B_\nu \phi(\nu) d\nu \\ &\simeq B_\nu \int_0^\infty \phi(\nu) d\nu \\ &\simeq B_\nu\end{aligned}\tag{6.24}$$

because B_ν is much broader than $\phi(\nu)$. We therefore write

$$\frac{A_{21}/B_{21}}{(g_1 B_{12}/g_2 B_{21})e^{\Delta E/kT_{\text{rad}}} - 1} = \frac{2h\nu_0^3/c^2}{e^{\Delta E/kT_{\text{rad}}} - 1},\tag{6.25}$$

or

$$\begin{aligned}A_{21} &= \frac{2h\nu_0^3}{c^2} B_{21} \\ g_1 B_{12} &= g_2 B_{21}.\end{aligned}\tag{6.26}$$

These relations are also valid in general.

We now slightly rewrite equation (6.1) with

$$I_\nu = I_\nu(0)e^{-\tau_\nu} + \frac{j_\nu}{\alpha_\nu}(1 - e^{-\tau_\nu}),\tag{6.27}$$

where we used the ratio of the emissivity j_ν and the absorption coefficient $\alpha_\nu = \rho\kappa_\nu$ (i.e., the inverse of the photon mean free path, with κ_ν is the opacity; see Sec. 2.2.2 in Chapter 2) in lieu of the source function S_ν . We use the Einstein coefficients to express

$$\begin{aligned}j_\nu &= \frac{h\nu}{4\pi} n_2 A_{21} \phi(\nu) \\ \alpha_\nu &= \frac{h\nu}{4\pi} (n_1 B_{12} - n_2 B_{21}) \phi(\nu)\end{aligned}\tag{6.28}$$

where it was assumed that the emission is isotropic. It is to be noted that the absorption coefficient contains a correction due to the presence of stimulated emission in the last of equations (6.28). Calculating the ratio j_ν/α_ν from equations (6.26) and (6.28) would lead us back to equation (6.25) (and to expressing the source function with Planck's law), as would be expected. We can, however, use our equation for the absorption coefficient

to express the optical depth as a function of the total **column density** $N \equiv n\Delta s$, where n is the total volume density of the molecule under study and Δs is the depth of the column of gas through the emitting region. We then find that

$$\begin{aligned}\tau_\nu &= \alpha_\nu \Delta s \\ &= \frac{h\nu}{4\pi} (n_1 B_{12} - n_2 B_{21}) \phi(\nu) \Delta s \\ &= \frac{c^2 A_{21}}{8\pi\nu^2} \frac{g_2}{g_1} (1 - e^{-\Delta E/kT_{\text{ex}}}) \phi(\nu) n_1 \Delta s,\end{aligned}\tag{6.29}$$

where we used equations (6.26) and the Boltzmann distribution

$$\frac{n_2}{n_1} = \frac{g_2}{g_1} e^{-\Delta E/kT_{\text{kin}}}.\tag{6.30}$$

It is also customary to approximate the density profile with a width representative for the line profile, i.e.,

$$\phi(\nu) \equiv \Delta\nu^{-1}.\tag{6.31}$$

Finally, we can link the density of the lower level n_1 to the total density n through the partition function U with

$$\begin{aligned}n &= \sum_{J=0}^{\infty} n_J \\ &= n_0 \sum_{J=0}^{\infty} \frac{n_J}{n_0} \\ &= n_0 \sum_{J=0}^{\infty} \frac{g_J}{g_0} e^{-\Delta E_{J0}/kT_{\text{ex}}} \\ &\equiv n_0 U.\end{aligned}\tag{6.32}$$

where we assumed that a single excitation temperature characterizes all possible transitions.

For the rotational levels of linear molecules like carbon monoxide and its isotopologues

$$\begin{aligned}\frac{g_J}{g_0} &= 2J + 1 \\ \Delta E_{J0} &= B_e \hbar^2 J(J+1) \\ &= \frac{1}{2} kT_0 (1 \rightarrow 0) J(J+1).\end{aligned}\tag{6.33}$$

Inserting these relations in equation (6.32) for the partition function we get (setting $J' = J + 1/2$)

$$\begin{aligned}
U_{\text{CO}} &= \sum_{J=0}^{\infty} (2J+1) e^{-T_0(1 \rightarrow 0)J(J+1)/2T_{\text{ex}}} \\
&\approx \int_0^{\infty} (2J+1) e^{-T_0(1 \rightarrow 0)J(J+1)/2T_{\text{ex}}} dJ \\
&\approx 2 \int_{1/2}^{\infty} J' e^{-T_0(1 \rightarrow 0)(J'^2 - 1/4)/2T_{\text{ex}}} dJ' \\
&\approx 2 e^{T_0(1 \rightarrow 0)/8T_{\text{ex}}} \int_{1/2}^{\infty} J' e^{-T_0(1 \rightarrow 0)J'^2/2T_{\text{ex}}} dJ' \\
&\approx 2 \frac{T_{\text{ex}}}{T_0}.
\end{aligned} \tag{6.34}$$

It follows from equations (6.29), (6.31), and (6.34) that, in general,

$$n_J \Delta s = \frac{8\pi\nu^2 \Delta\nu\tau_v}{c^2 A_{J+1,J}} \left(\frac{g_J}{g_{J+1}} \right) \left(1 - e^{-\Delta E_{J+1,J}/kT_{\text{ex}}} \right)^{-1}. \tag{6.35}$$

But since $n_J = n_0 (n_J/n_0) = (n/U)(n_J/n_0) = (n/U)(g_J e^{-\Delta E_{J0}/kT_{\text{ex}}}/g_0)$, we can write

$$N = \frac{16\pi\nu^2 \Delta\nu\tau_v}{c^2 A_{J+1,J}} \cdot \frac{g_0}{g_{J+1}} \cdot \frac{T_{\text{ex}}}{T_0(1 \rightarrow 0)} \left(\frac{e^{\Delta E_{J0}/kT_{\text{ex}}}}{1 - e^{-\Delta E_{J+1,J}/kT_{\text{ex}}}} \right). \tag{6.36}$$

We now go back to the spectra of Figure 6-1 and seek to evaluate the column densities of $^{12}\text{C}^{18}\text{O}$ and $^{13}\text{C}^{16}\text{O}$. To do so we need the following quantities for $J = 1$ with $^{12}\text{C}^{18}\text{O}$

$$\begin{aligned}
\nu_0 &= 219.6 \text{ GHz} \\
\Delta\nu &= \Delta V \left(\frac{\nu_0}{c} \right) \approx 4 \text{ km s}^{-1} \left(\frac{\nu_0}{c} \right) \approx 2.93 \text{ MHz} \\
\frac{\Delta E}{k} &= T_0(2 \rightarrow 1) = 10.6 \text{ K} \\
\frac{\Delta E_{10}}{k} &= T_0(1 \rightarrow 0) \\
T_0(1 \rightarrow 0) &\approx \frac{10.6 \text{ K}}{2} = 5.3 \text{ K}.
\end{aligned} \tag{6.37}$$

Inserting equations (6.37) into equation (6.36) we get

$$N(^{12}\text{C}^{18}\text{O}) = 3.26 \times 10^{16} \text{ cm}^{-2}. \tag{6.38}$$

It follows that the column density for $^{13}\text{C}^{16}\text{O}$ is

$$\begin{aligned} N(^{13}\text{C}^{16}\text{O}) &= N_{\text{tot}}(^{12}\text{C}^{18}\text{O}) \left[\frac{^{12}\text{C}}{^{13}\text{C}} \right]^{-1} \left[\frac{^{16}\text{O}}{^{18}\text{O}} \right] \\ &= 1.5 \times 10^{17} \text{ cm}^{-2}. \end{aligned} \quad (6.39)$$

Where we used the relevant isotopic ratios for the DR21(OH) molecular cloud, i.e.,

$$\begin{aligned} \left[\frac{^{12}\text{C}}{^{13}\text{C}} \right] &= 66 \\ \left[\frac{^{16}\text{O}}{^{18}\text{O}} \right] &= 312. \end{aligned} \quad (6.40)$$

Although considering such an analysis would require going into more details than is possible here, the hydrogen column density can be inferred from $^{13}\text{C}^{16}\text{O}$ measurements. Briefly stated, since we already derived a connection between N_{H} and A_{V} from equation (2.47) in Chapter 2 with

$$\frac{N_{\text{H}}}{A_{\text{V}}} = 1.9 \times 10^{21} \text{ mag}^{-1} \text{ cm}^{-2}, \quad (6.41)$$

the mapping of A_{V} for stars located behind molecular clouds that are not too opaque, while using corresponding measurements of the column density $N(^{13}\text{C}^{16}\text{O})$ for these same clouds (as per in equation (6.36) and (6.39), for example) allows one to establish an empirical connection between N_{H} and $N(^{12}\text{C}^{18}\text{O})$. It is then found that

$$\frac{N(^{13}\text{C}^{16}\text{O})}{A_{\text{V}}} = 2.5 \times 10^{15} \text{ mag}^{-1} \text{ cm}^{-2}, \quad (6.42)$$

and from equation (6.41) we have

$$N_{\text{H}} = 7.5 \times 10^5 N(^{13}\text{C}^{16}\text{O}). \quad (6.43)$$

Applying equation (6.43) to DR21(OH), using equation (6.39), yields

$$N_{\text{H}} \approx 1.1 \times 10^{23} \text{ cm}^{-2}. \quad (6.44)$$