

**ASTR 5110 Atomic and Molecular Processes Fall 2023. Problem Set 11. Due
Wed 6 Dec.**

1. Carbon Monoxide

Sagittarius B2 is a giant molecular cloud some 120 pc from the Galactic Center. It is one of the most massive ($\sim 6 \times 10^6 M_{\odot}$) and active star-forming regions in the Galaxy, with a rich molecular spectrum. The cloud is considered to be a possible prototype for vigorous star-forming regions in other galaxies such as M82 and Arp 220.

Figure 1 shows a Herschel infrared image of Sgr B2, and Figure 3 shows Herschel spectra of the North (N) and Middle (M) molecular cores, and of the overall region (Etxaluze et al. 2013, arXiv:1307.0335 <https://arxiv.org/abs/1307.0335>). The spectra show infrared fine structure emission lines of [C I], emission lines of CO and some other molecules, and absorption lines of yet other molecules. The absorption lines probably arise from absorption by cool molecular gas along the line of sight through the Galactic disk to Sgr B2.

(a) (4 points) The lowest allowed rotational transition of CO, the transition $\text{CO } X^1\Sigma^+(v=0-0)(J=1-0)$, is at wavelength 0.2601 cm in the radio (Table 1B of Morton & Noreau 1994, Ap. J. Supp. 95, 301). The energy level of the J 'th rotational energy is $E_J = BJ(J + 1)$ relative to the $J = 0$ level. Calculate the rotational constant B in Kelvin.

(b) (4 points) What is the reduced mass of the isotopic molecule ^{13}CO relative to that of CO? Explain why this ratio is all that is needed to deduce the relative wavelengths of the rotational transitions of ^{13}CO relative to CO. Deduce the wavelength of the $J = 1-0$ rotational transition of ^{13}CO , and the corresponding rotational constant B_{13} .

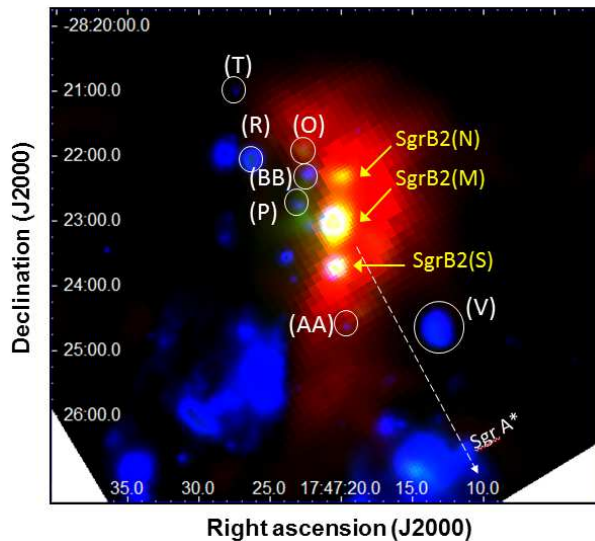


Figure 1: Composite infrared Herschel image of the Sgr B2 molecular cloud at $24 \mu\text{m}$ (blue), $70 \mu\text{m}$ (green), and $350 \mu\text{m}$ (red), showing the three main star-forming molecular cores North (N), Middle (M), and South (S). The bluish blobs trace HII regions around hot young stars. The white dashed arrow points at the direction of Sgr A* at the Galactic Center. This is Figure 5 of Etxaluze et al. (2013).

(c) (No credit). The electric dipole spontaneous transition probability A_{UL} from upper state U to lower state L is, equation (2.11) in the notes on Selection Rules,

$$A_{UL} = \frac{4\omega^3}{3c^3\hbar} |\langle U|\mathbf{d}|L\rangle|^2 = \frac{4(2\pi)^3}{3\lambda^3\hbar} |\langle U|\mathbf{d}|L\rangle|^2 . \quad (1.1)$$

For rotational transitions, the dipole matrix element $\langle U|\mathbf{d}|L\rangle$ is a product of a factor that depends on the upper and lower electronic and vibrational states and is independent of the rotational state, and a factor that depends on the rotational state. In the present case, where CO is in its ground electronic and vibrational state, the electronic/vibrational dipole factor is the permanent dipole moment of CO (a.u. \equiv atomic unit),

$$|\mathbf{d}_{\text{perm}}| = 0.0441 \text{ a.u.} . \quad (1.2)$$

Note that permanent dipole moments are commonly quoted in Debye units (D), in terms of which $1 \text{ a.u.} = \hbar^2/m_e e = 2.5417465 \times 10^{-18} \text{ gm}^{1/2} \text{ cm}^{5/2} \text{ s}^{-1} = 2.5417465 \text{ D}$. The transition probability of a rotational transition in the ground electronic/vibrational state is then (recall that Hönl-London factors are defined as a sum over upper and lower rotational states, so the transition probability $g_U A_{UL}$ here includes the statistical weight factor g_U of the upper level)

$$g_U A_{UL} = \frac{4(2\pi)^3}{3\lambda_{UL}^3\hbar} f(U|L) |\mathbf{d}_{\text{perm}}|^2 , \quad (1.3)$$

where the relevant Hönl-London factor $f(U|L)$ is equation (1.9a) in the notes on Hönl-London factors, with $K = J$ and $\Lambda = 0$,

$$f(U|L) = f(J_U, \Lambda_U | J_L, \Lambda_L) = f(J + 1, 0 | J, 0) = J + 1 = J_U . \quad (1.4)$$

The lowest rotational transition, $1 \rightarrow 0$, has a wavelength of 0.2601 cm , which is $4.915 \times 10^7 \text{ a.u.}$ The spontaneous transition probability $g_1 A_{10}$ of the lowest rotational transition is, in atomic units, with $g_1 = 3$,

$$g_1 A_{10} = \frac{4(2\pi)^3}{3(4.915 \times 10^7)^3} \cdot (0.0441)^2 \text{ a.u.} = 5.42 \times 10^{-24} \text{ a.u.} , \quad (1.5)$$

or in mks units

$$g_1 A_{10} = 2.24 \times 10^{-7} \text{ s}^{-1} . \quad (1.6)$$

(d) (4 points) Argue that, if the rotational levels are populated in statistical (i.e. relative thermodynamic) equilibrium at temperature T , then the intensities of the rotational lines, integrated over their line profiles, will be proportional to

$$I_{UL} \propto g_U A_{UL} E_{UL} e^{-E_U/kT} . \quad (1.7)$$

(e) (4 points) Argue from the dipole formula (1.3) and the Hönl-London factors (1.4) that

$$g_U A_{UL} E_{UL} \propto E_{UL}^5 \propto J_U^5 . \quad (1.8)$$

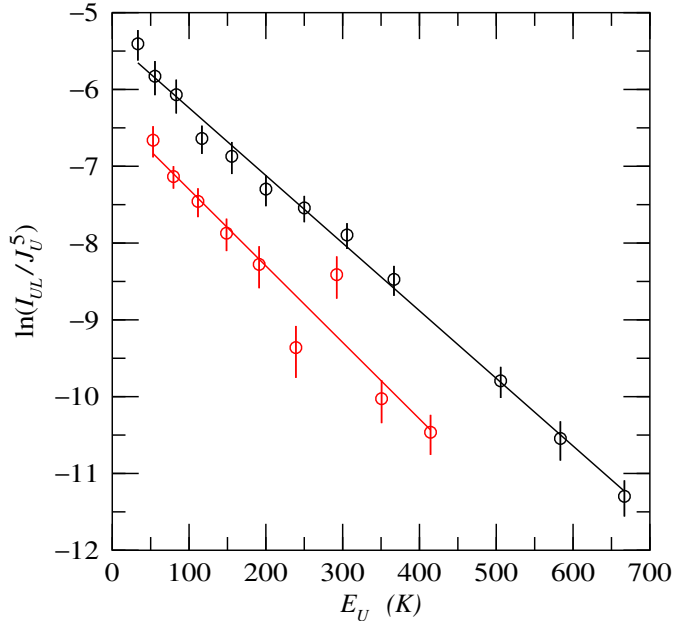


Figure 2: CO rotational diagram for the Sgr B2(M) region. The upper points with error bars (black) are for ^{12}CO , the lower (red) for ^{13}CO . Data are from Table 1 of Etzaluze et al. (2013). The straight lines are least squares fits through the points, with $\chi^2/\text{dof} = 6/10$ for CO, and $\chi^2/\text{dof} = 14/7$ for ^{13}CO .

(f) (4 points) Figure 2 shows a “rotational diagram” of the CO lines from the Sgr B2(M) region, a plot of $\ln(I_{UL}/J_U^2)$ versus E_U . Are the observed intensities consistent with the levels being in statistical equilibrium? From the rotational diagram, deduce the excitation temperature T in Kelvin of the CO lines. Explain what you did.

(g) (4 points) Suppose that the rotational states of the ground electronic/vibrational level are populated in statistical equilibrium, but that the excited electronic/vibrational states are all empty. Show that the partition function of the internal states of the CO molecule is approximately

$$\sum_{J=0}^{\infty} g_J e^{-E_J/kT} \approx \frac{T}{B} \quad (1.9)$$

for $T \gg B$. Is this condition satisfied in Sgr B2? [Hint: the condition $T \gg B$ allows you to replace the sum over states by an integral.]

(h) (4 points) A typical CO spectrum is far less rich than that of the Sgr B2 cloud. Often, the only line observed is the $J = 1 \rightarrow 0$ transition. Show that under the circumstances of part (g), and provided that the line is optically thin, the luminosity in the CO 1–0 line is approximately proportional to M_{CO}/T where M_{CO} is the mass of CO, and T is the excitation temperature of the CO. [Hint: Recall that, in thermodynamic equilibrium, the fraction of molecules in level J is $n_J/n_{\text{CO}} = g_J e^{-E_J/kT} / Z(T)$ where $Z(T)$ is the partition function.]

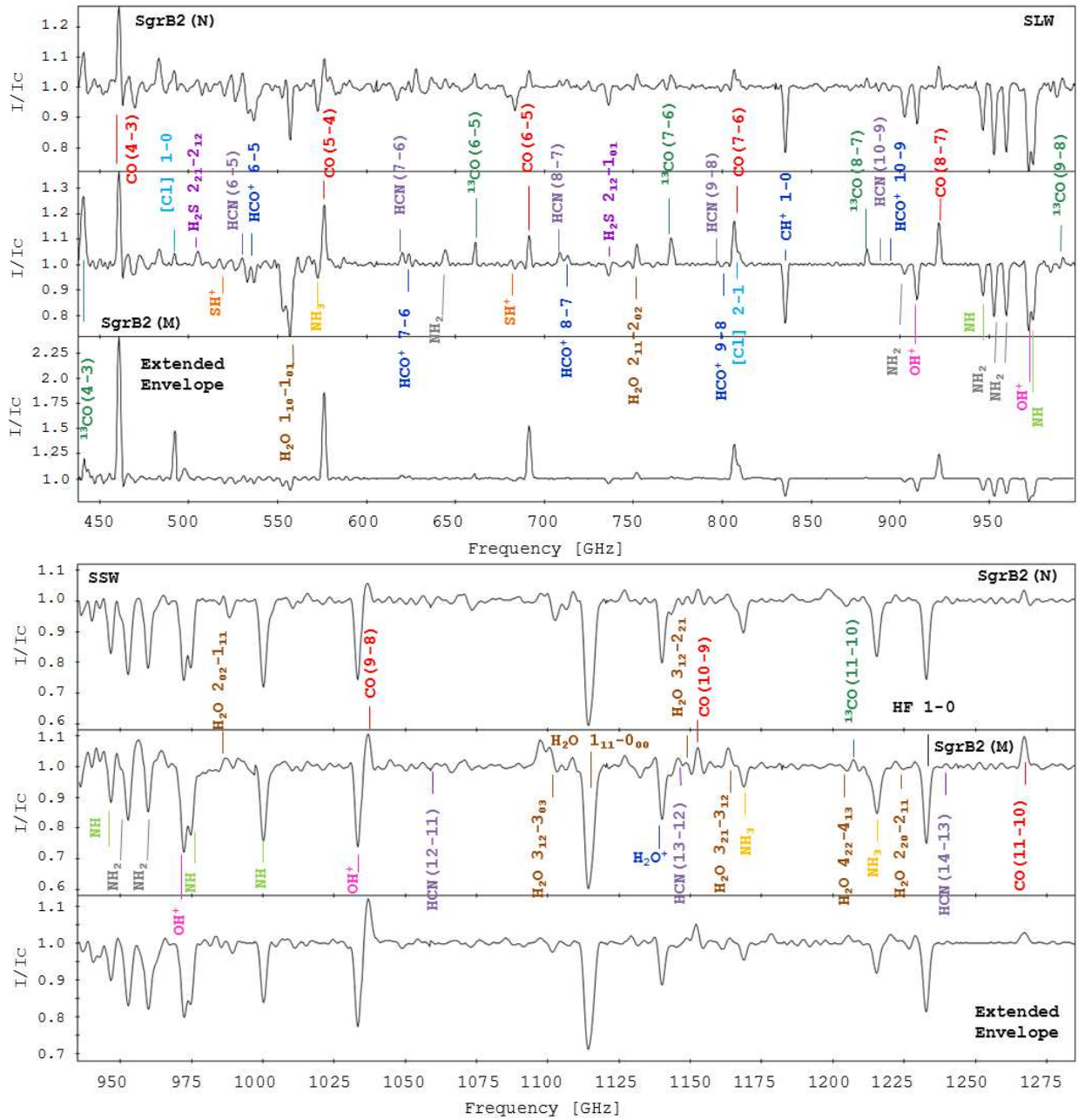


Figure 3: Herschel spectra of the North and Middle cores, and of the overall region, of the Sgr B2 molecular cloud (Etxaluze et al. 2013).