

**Astrophysics — ASTR-4220**  
**Class 28**  
**Molecular Spectra**

**Exercise (40 pts)**

Consider the rigid rotor model of a diatomic molecule, in which the nuclei rotate about their center of mass with a constant internuclear distance  $r_0$ . Let  $m_1$  and  $m_2$  be the masses of the two nuclei.

**1. (10 pts)** — Show that the inertia for rotation about the center of mass is  $I = m_r r_0^2$ , where  $m_r$  is the reduced mass.

**2. (10 pts)** — Show that the rotational kinetic energy  $E_{\text{rot}}$  is quantized such that

$$E_{\text{rot}} = B J(J + 1), \quad J = 0, 1, \dots, \quad (1)$$

where

$$B = \frac{\hbar^2}{2m_r r_0^2}. \quad (2)$$

**3. (10 pts)** — For the  $\text{H}_2$  molecule, even- $J$  levels can only decay radiatively to even- $J$  levels and similarly for odd levels. In addition, the quantum number  $J$  can only change by  $\Delta J = 0, \pm 2$ . What rotational emission line of  $\text{H}_2$  has the longest wavelength? Give the upper and lower values of  $J$  and the wavelength in microns.

**4. (10 pts)** — Repeat for the  $\text{CO}$  molecule noting that for heteronuclear molecules the selection rule is  $\Delta J = 0, \pm 1$ .

**Solution**

**1.** — Let  $r_1$  and  $r_2$  be the distances of mass 1 and 2, respectively, from the center of mass. Starting from  $m_1 r_1 = m_2 r_2$  it is easy to show that

$$r_1 = \frac{m_r}{m_1} r_0 \quad (3)$$

and

$$r_2 = \frac{m_r}{m_2} r_0. \quad (4)$$

It follows that

$$I = m_1 r_1^2 + m_2 r_2^2 = m_r r_0^2. \quad (5)$$

**2.** — The rotational energy is

$$E_{\text{rot}} = \frac{L^2}{2I} = \frac{J(J + 1)\hbar^2}{2m_r r_0^2}, \quad (6)$$

where  $L^2 = J(J + 1)\hbar^2$  is the quantized angular momentum squared. Then

$$E_{\text{rot}} = BJ(J + 1) \quad (7)$$

where

$$B = \frac{\hbar^2}{2m_{\text{r}}r_0^2}. \quad (8)$$

**3.** — The transition with the smallest energy difference is  $J = 2 \rightarrow 0$  for which  $\Delta E = 6B$ . The wavelength is

$$\lambda = \frac{hc}{\Delta E} = 27\mu\text{m}, \quad (9)$$

where Table 5.1 has been used.

**4.** — The transition is  $J = 1 \rightarrow 0$  with  $\Delta E = 2B$  and  $\lambda = 2.6$  mm.