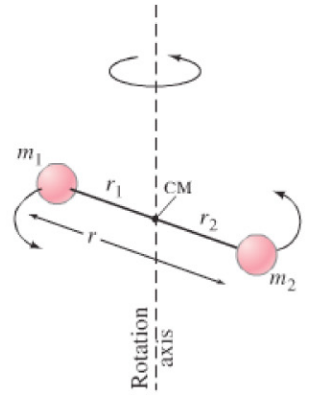


FIGURE 29–15 Diatomic molecule rotating about a vertical axis.

* Rotational Energy Levels in Molecules

We consider only diatomic molecules, although the analysis can be extended to polyatomic molecules. When a diatomic molecule rotates about its center of mass as shown in Fig. 29–15, its kinetic energy of rotation (see Section 8–7) is

$$E_{\text{rot}} = \frac{1}{2} I\omega^2 = \frac{(I\omega)^2}{2I},$$

where $I\omega$ is the angular momentum (Section 8–8). Quantum mechanics predicts quantization of angular momentum just as in atoms (see Eq. 28–3):

$$I\omega = \sqrt{L(L+1)}\,\hbar, \qquad L = 0, 1, 2, \cdots,$$

where L is an integer called the **rotational angular momentum quantum number**. Thus the rotational energy is quantized:

$$E_{\text{rot}} = \frac{(I\omega)^2}{2I} = L(L+1)\frac{\hbar^2}{2I}, \qquad L = 0, 1, 2, \cdots. \tag{29–1}$$

Selection rule (rotational levels)

Transitions between rotational energy levels are subject to the *selection rule* (as in Section 28–6):

$$\Delta L = \pm 1.$$

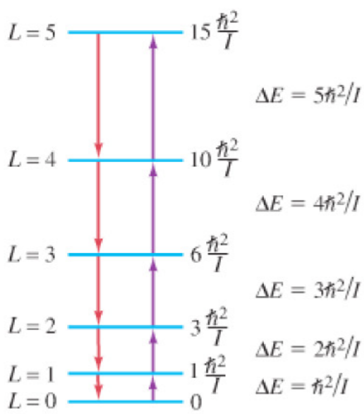
The energy of a photon emitted or absorbed for a transition between rotational states with angular momentum quantum number L and $L-1$ will be

$$\Delta E_{\text{rot}} = E_L - E_{L-1} = \frac{\hbar^2}{2I} L(L+1) - \frac{\hbar^2}{2I}(L-1)(L)$$

$$= \frac{\hbar^2}{I} L. \qquad \left[\begin{array}{l} L \text{ is for upper} \\ \text{energy state} \end{array}\right] \tag{29–2}$$

We see that the transition energy increases directly with L. Figure 29–16 shows some of the allowed rotational energy levels and transitions. Measured absorption lines fall in the microwave or far-infrared regions of the spectrum, and their frequencies are generally 2, 3, 4, ⋯ times higher than the lowest one, as predicted by Eq. 29–2.

FIGURE 29–16 Rotational energy levels and allowed transitions (emission and absorption) for a diatomic molecule. Upward-pointing arrows represent absorption of a photon, and downward arrows represent emission of a photon.



EXAMPLE 29–2 Rotational transition. A rotational transition $L = 1$ to $L = 0$ for the molecule CO has a measured absorption wavelength $\lambda_1 = 2.60\,\text{mm}$ (microwave region). Use this to calculate (*a*) the moment of inertia of the CO molecule, and (*b*) the CO bond length, r.

APPROACH The absorption wavelength is used to find the energy of the absorbed photon, and we can then calculate the moment of inertia, I, from Eq. 29–2. The moment of inertia is related to the CO separation (bond length r).

SOLUTION (*a*) The photon energy, $E = hf = hc/\lambda$, equals the rotational energy level difference, ΔE_{rot}. From Eq. 29–2, we can write

$$\frac{\hbar^2}{I} L = \Delta E_{\text{rot}} = hf = \frac{hc}{\lambda_1}.$$

With $L = 1$ (the upper state) in this case, we solve for I:

$$I = \frac{\hbar^2 L}{hc}\lambda_1 = \frac{h\lambda_1}{4\pi^2 c} = \frac{(6.63 \times 10^{-34}\,\text{J}\cdot\text{s})(2.60 \times 10^{-3}\,\text{m})}{4\pi^2(3.00 \times 10^8\,\text{m/s})}$$

$$= 1.46 \times 10^{-46}\,\text{kg}\cdot\text{m}^2.$$

(*b*) The molecule rotates about its center of mass (CM) as shown in Fig. 29–15. Let m_1 be the mass of the C atom, $m_1 = 12\,\text{u}$, and let m_2 be the mass of the O, $m_2 = 16\,\text{u}$. The distance of the CM from the C atom, which is r_1 in Fig. 29–15, is given by the CM formula, Eq. 7–9:

$$r_1 = \frac{0 + m_2 r}{m_1 + m_2} = \frac{16}{12 + 16} r = 0.57r.$$

The O atom is a distance $r_2 = r - r_1 = 0.43r$ from the CM. The moment of