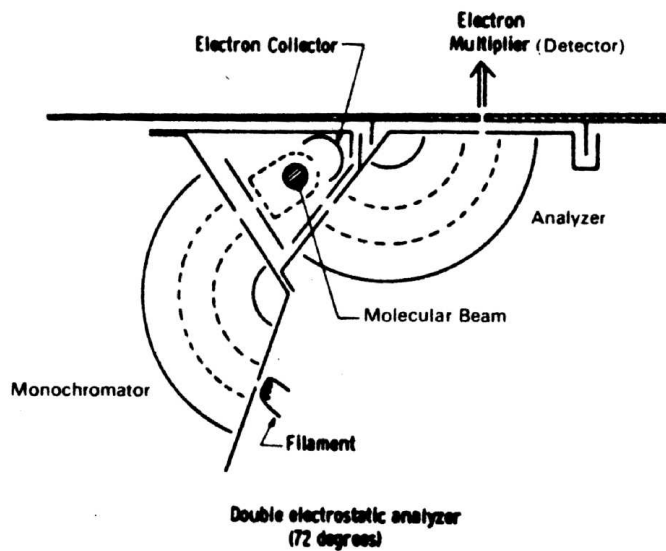
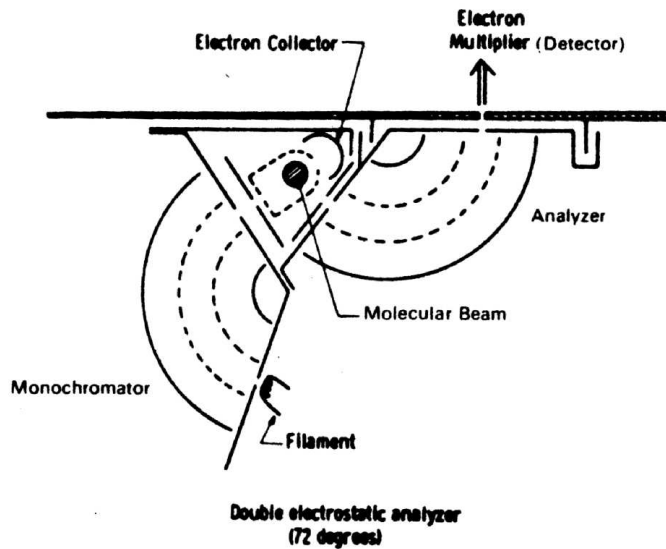


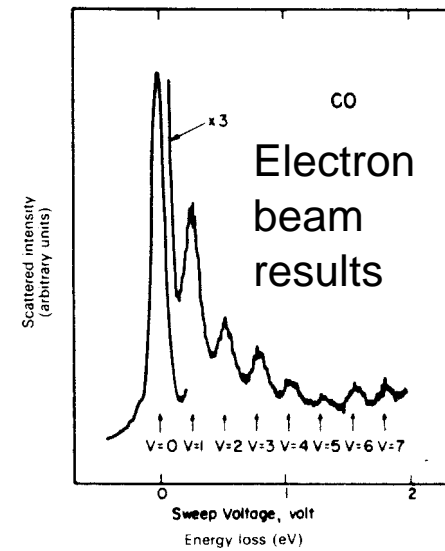
Fun With Carbon Monoxide



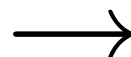
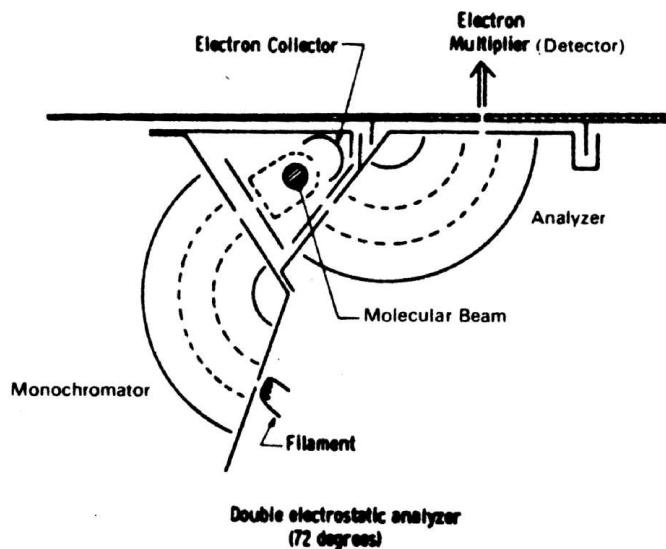
Fun With Carbon Monoxide



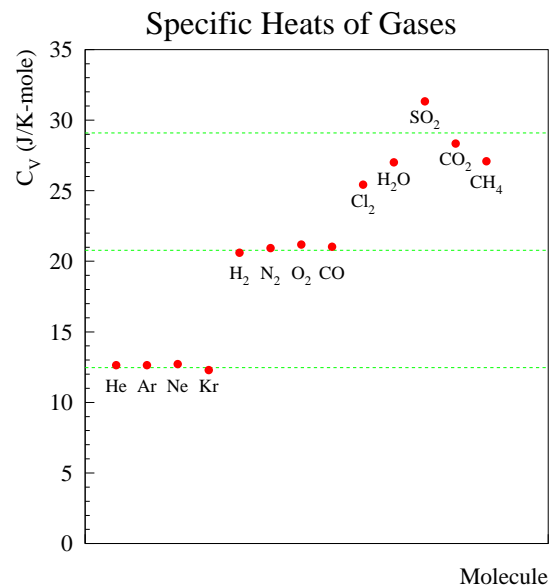
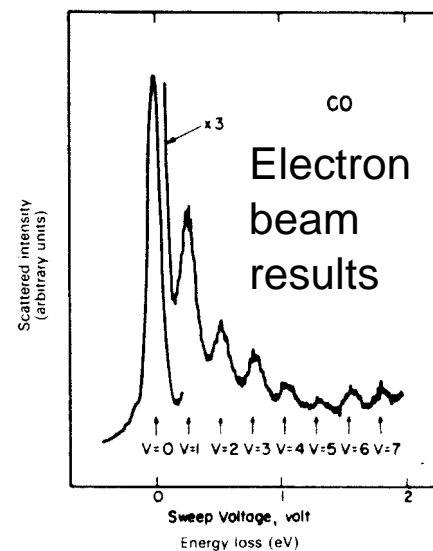
$$\Delta E = 0.25 \pm 0.05 \text{ eV}$$



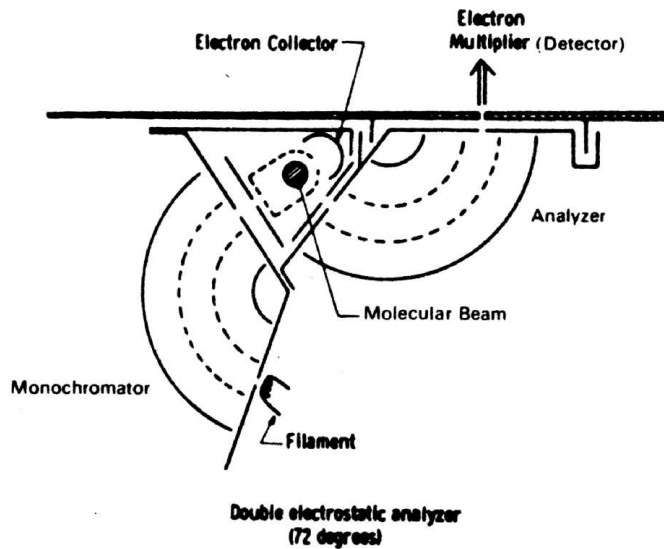
Fun With Carbon Monoxide



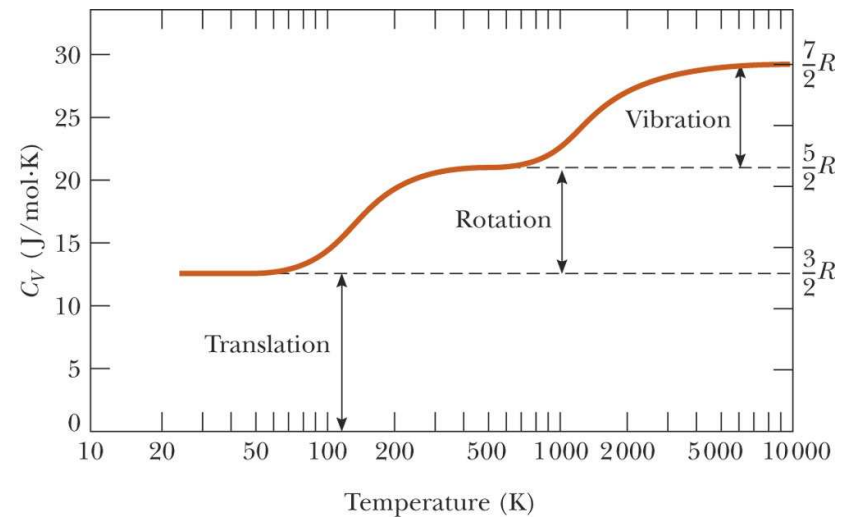
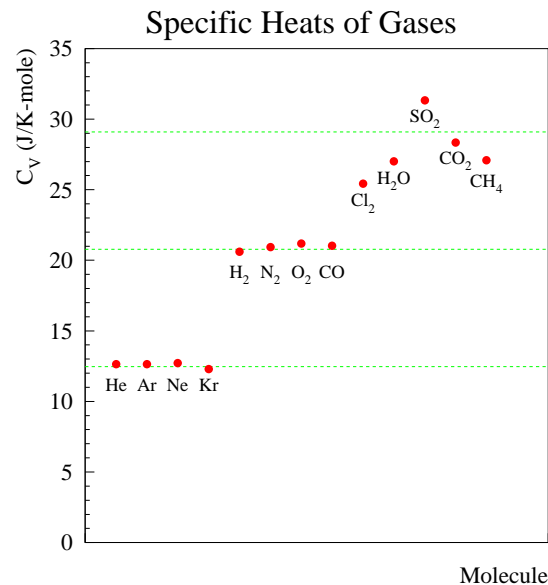
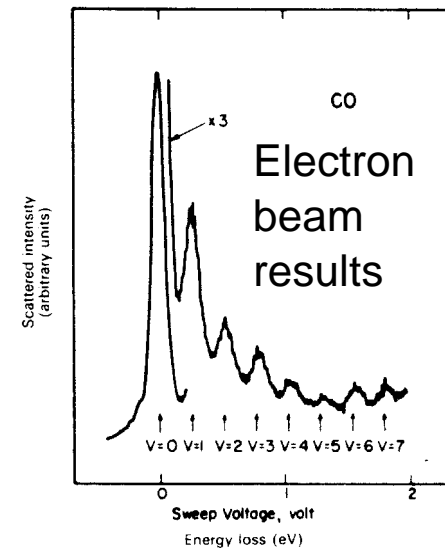
$$\Delta E = 0.25 \pm 0.05 \text{ eV}$$



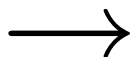
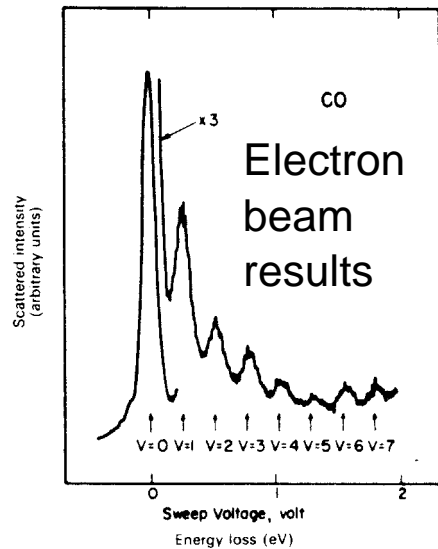
Fun With Carbon Monoxide



$$\Delta E = 0.25 \pm 0.05 \text{ eV}$$



Carbon Monoxide



$$\Delta E = 0.25 \pm 0.05 \text{ eV}$$

CO Absorption Spectrum

Incident light

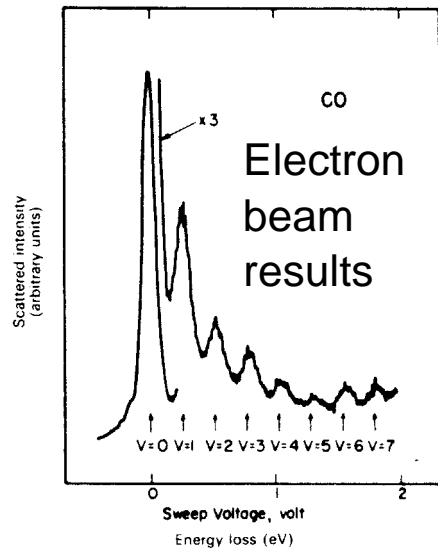


CO gas target



Photon detector

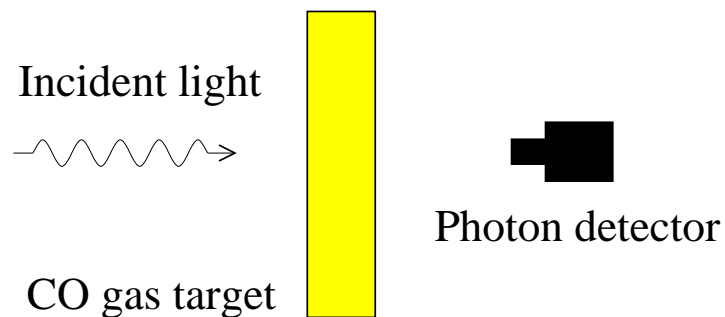
Carbon Monoxide



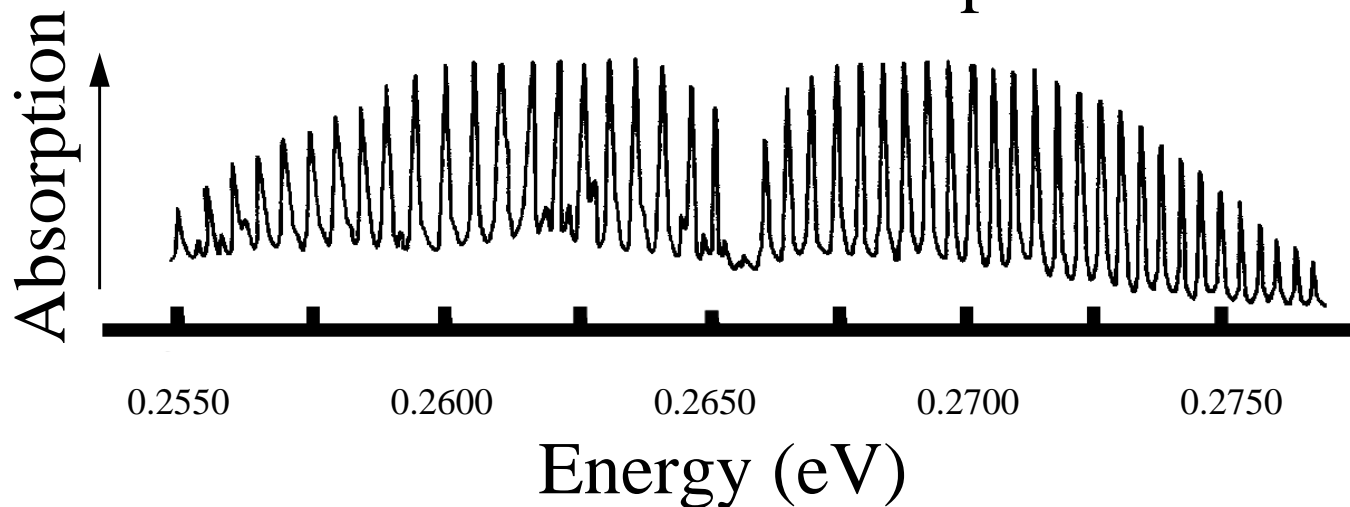
→

$$\Delta E = 0.25 \pm 0.05 \text{ eV}$$

CO Absorption Spectrum



Carbon-Monoxide Spectrum



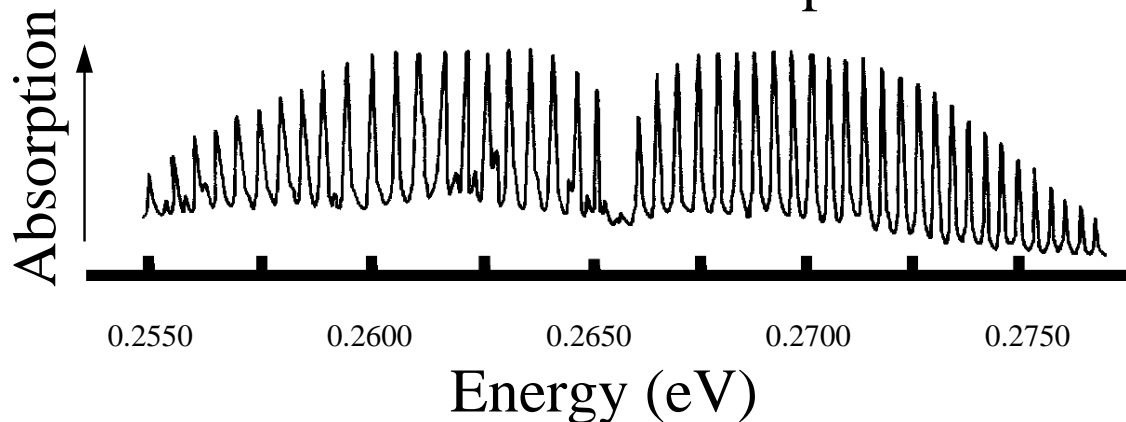
Is Carbon Monoxide A Rigid Rotator?

Excited states of carbon monoxide (CO) can be observed by passing light through a cell containing CO and measuring the absorption spectrum shown below. The molecule can both vibrate and rotate at the same time. The rotational energy states of a rigid rotator are

$$E_l = \frac{\hbar^2}{2I}l(l + 1)$$

where I is the moment of inertia. The vibrational part of the energy can be described by the harmonic oscillator so $E_n = (n + \frac{1}{2})\hbar\omega_0$ with $\Delta E = \hbar\omega_0 = 0.25 \pm 0.05 \text{ eV}$. How does one arrive at the expression above for the rotational energy? Is CO a rigid rotator?

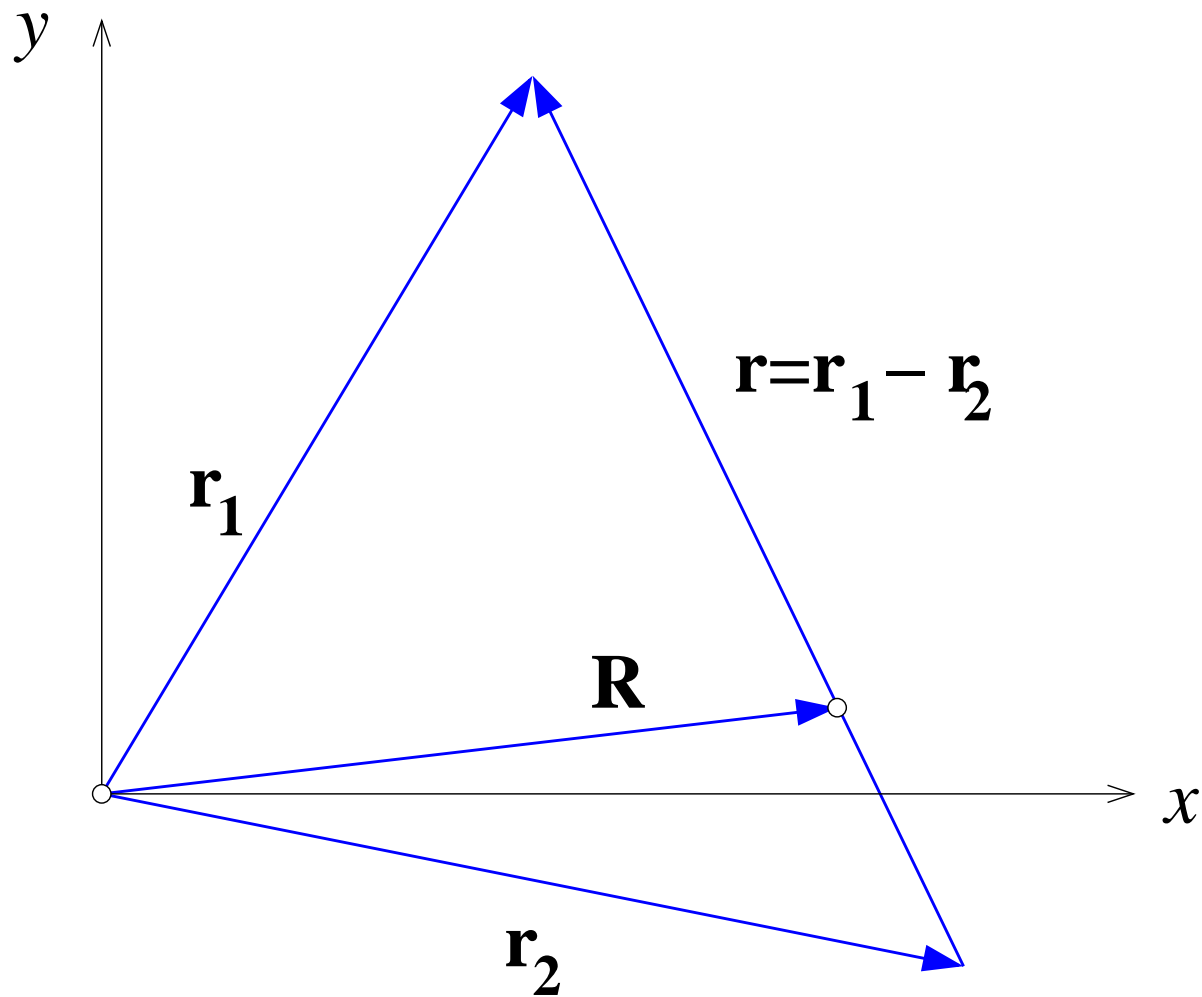
Carbon–Monoxide Spectrum



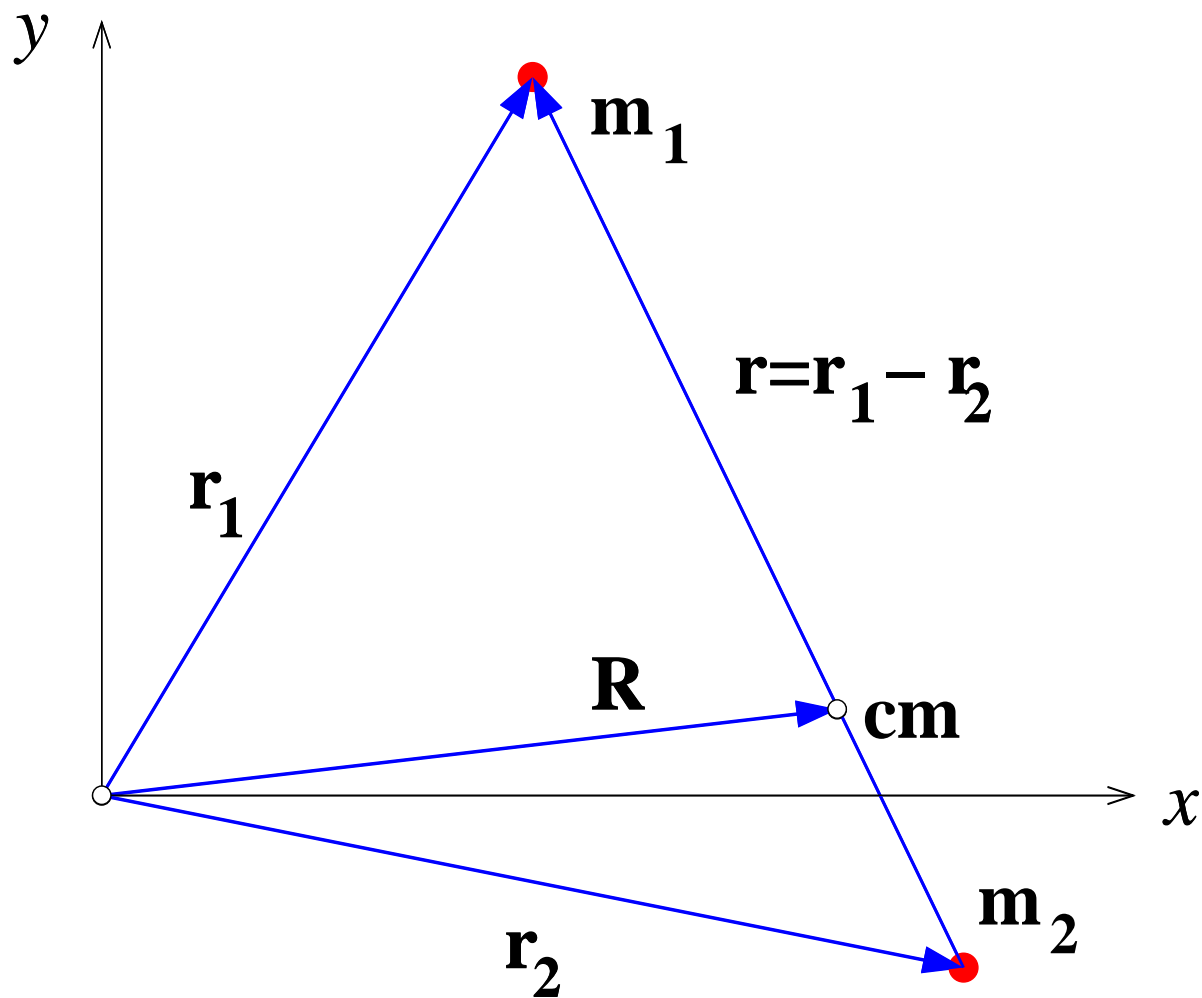
The Plan

1. What is the kinetic and potential energy between the carbon and oxygen atoms in CO in the CM frame in cartesian and spherical coordinates?
2. How do you decompose the kinetic energy into radial and angular parts?
3. What is the Schroedinger equation for the rigid rotator?
4. What is the solution of the rigid rotator Schroedinger equation?

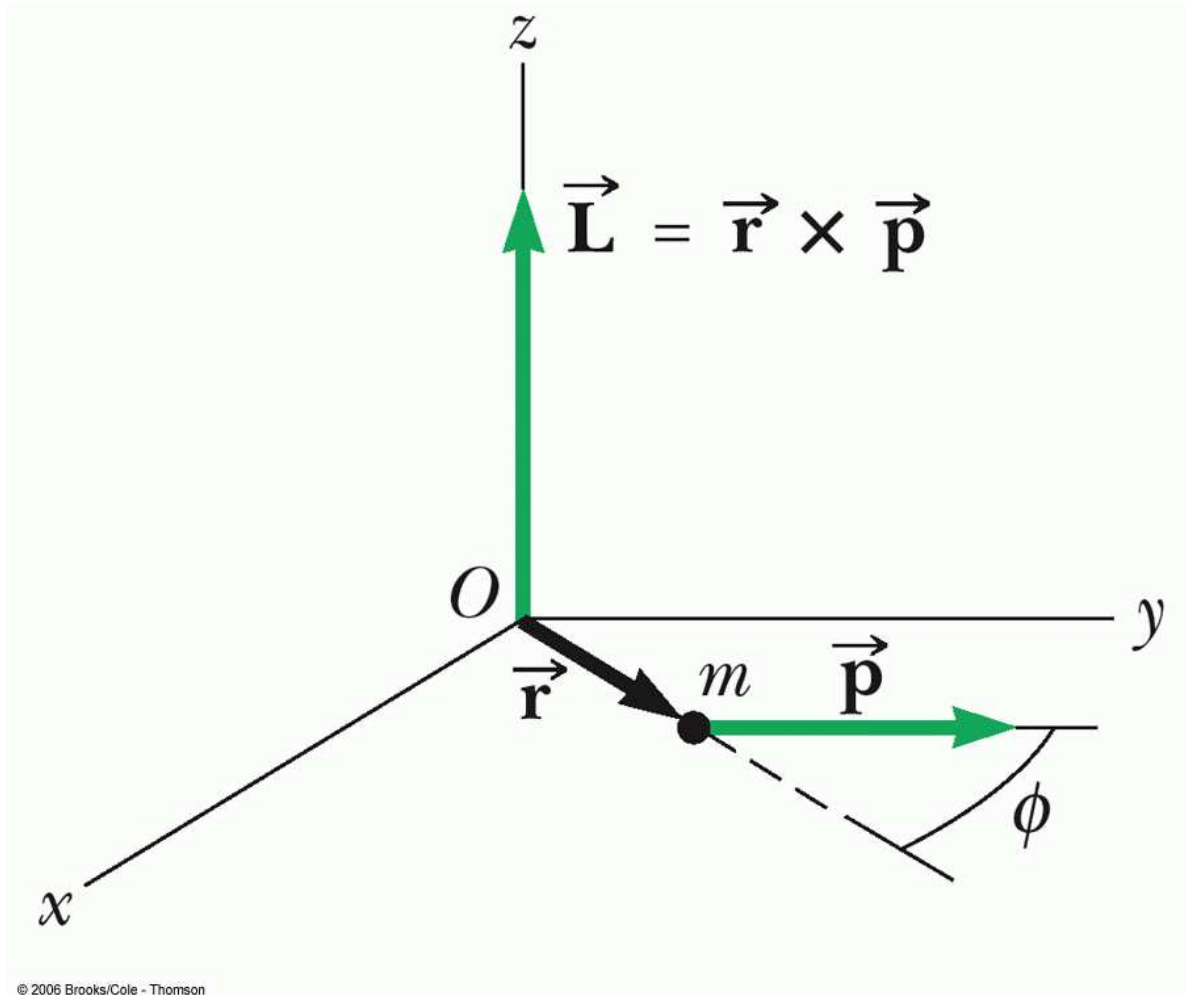
Coordinates



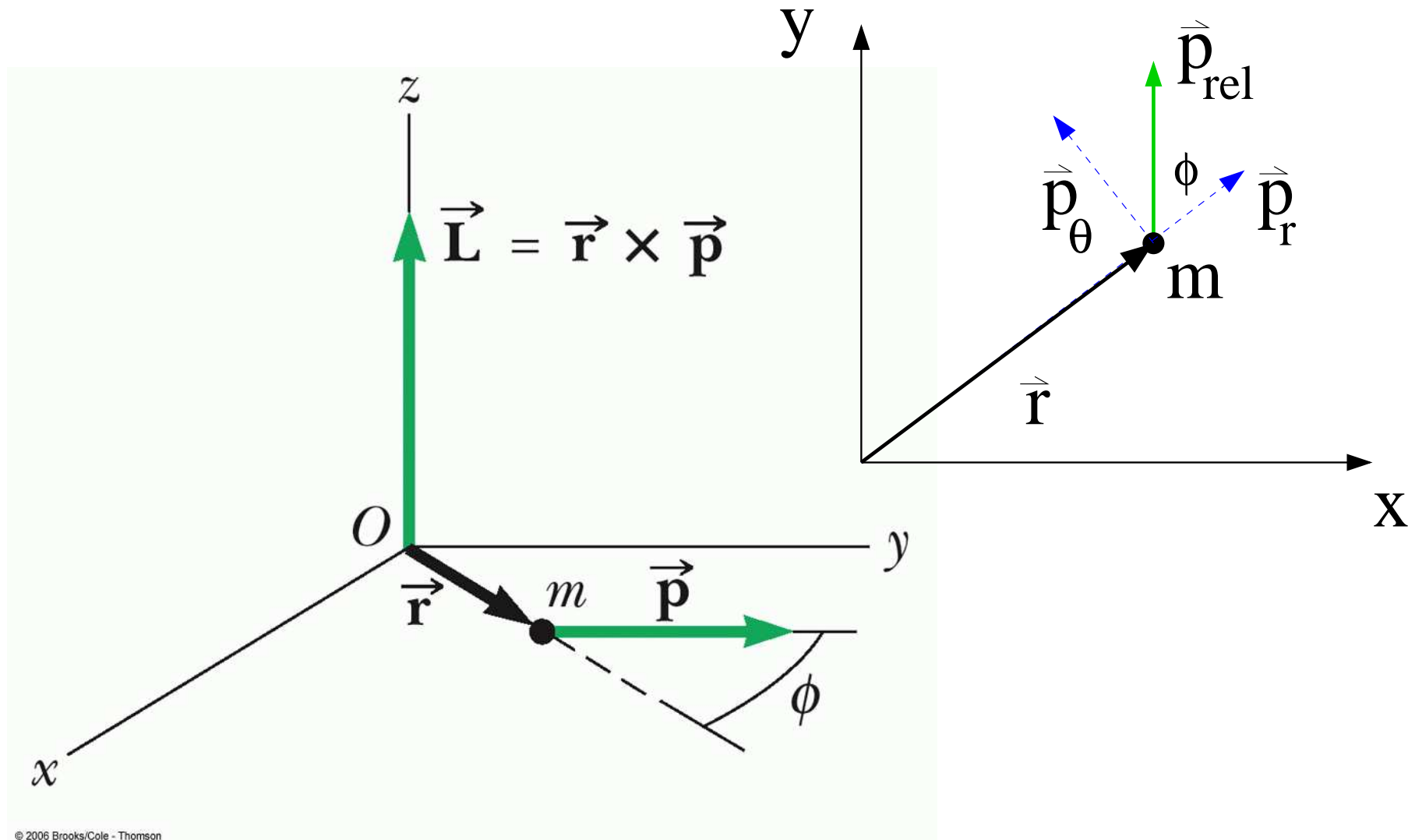
Coordinates



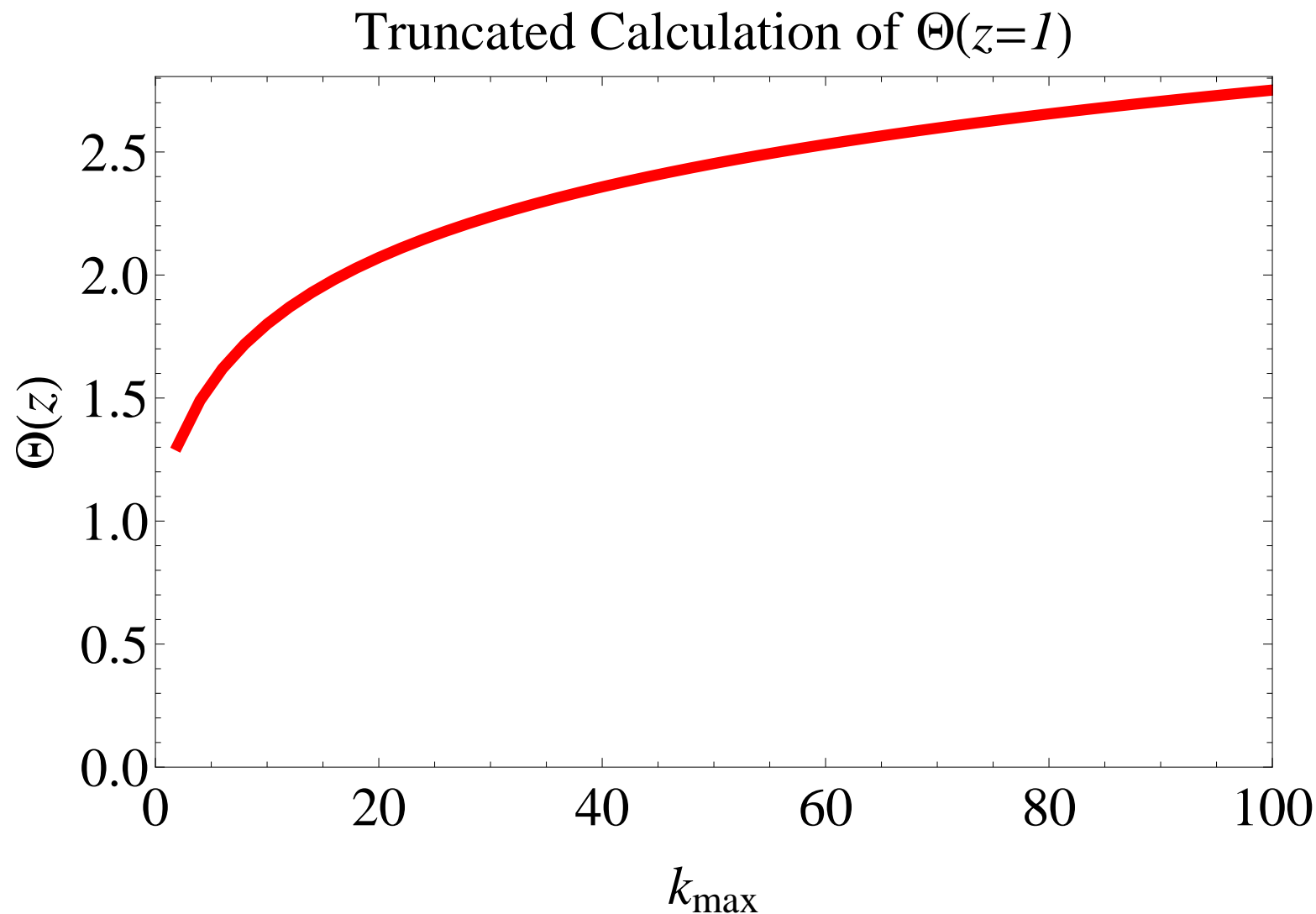
Angular Momentum



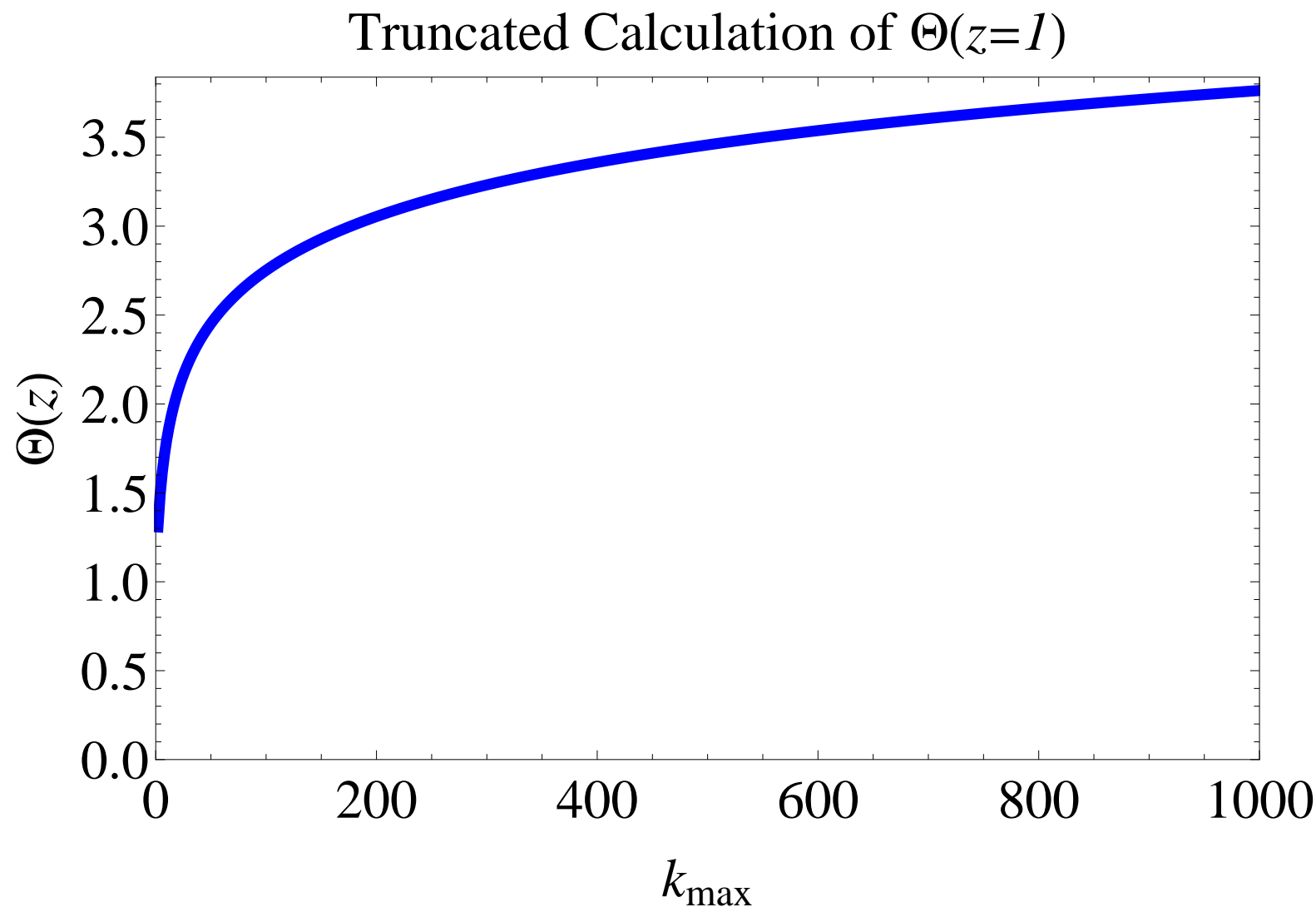
Angular Momentum



A Convergence Problem



A Convergence Problem



Legendre Polynomials ($m_l = 0$)

$$\Theta(\theta) = P_l(\cos \theta)$$

$$P_0(\cos \theta) = 1$$

$$P_1(\cos \theta) = \cos \theta$$

$$P_2(\cos \theta) = \frac{1}{2} (3 \cos^2 \theta - 1)$$

$$P_3(\cos \theta) = \frac{1}{2} (5 \cos^3 \theta - 3 \cos \theta)$$

Spherical Harmonics ($m_l = m$)

$$\Theta(\theta)\Phi(\phi) = Y_l^m(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi}$$

$$Y_0^0(\theta, \phi) = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^1(\theta, \phi) = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi} \quad Y_1^{-1}(\theta, \phi) = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}$$

$$Y_1^0(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos\theta$$

Summary So Far

$$\frac{p_r^2}{2\mu} = -\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$$

$$\frac{L^2}{2\mu r^2} = -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

$$m_l = 0, \pm \frac{1}{2}, \pm \frac{2}{2}, \pm \frac{3}{2}, \pm \frac{4}{2}, \pm \frac{5}{2}, \dots$$

$$\left[-\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{m_l^2}{\sin^2 \theta} \right] \Theta = A \Theta \quad A = l(l+1)$$

$$L^2 |\phi_s\rangle = \hbar^2 l(l+1) |\phi_s\rangle$$

The Eigenvalues of \hat{L}^2 and \hat{L}_z

$$\begin{aligned}\vec{L} &= \vec{r} \times \vec{p} \\ &= L_x \hat{i} + L_y \hat{j} + L_z \hat{k}\end{aligned}$$

The Eigenvalues of \hat{L}^2 and \hat{L}_z

$$\vec{L} = \vec{r} \times \vec{p}$$

$$= L_x \hat{i} + L_y \hat{j} + L_z \hat{k}$$

$$= (yp_z - zp_y) \hat{i} + (zp_x - xp_z) \hat{j} + (xp_y - yp_x) \hat{k}$$

The Eigenvalues of \hat{L}^2 and \hat{L}_z

$$\begin{aligned}\vec{L} &= \vec{r} \times \vec{p} \\ &= L_x \hat{i} + L_y \hat{j} + L_z \hat{k} \\ &= (yp_z - zp_y) \hat{i} + (zp_x - xp_z) \hat{j} + (xp_y - yp_x) \hat{k} \\ &= \frac{\hbar}{i} \left[\left(y \frac{d}{dz} - z \frac{d}{dy} \right) \hat{i} + \left(z \frac{d}{dx} - x \frac{d}{dz} \right) \hat{j} + \left(x \frac{d}{dy} - y \frac{d}{dx} \right) \hat{k} \right]\end{aligned}$$

The Eigenvalues of \hat{L}^2 and \hat{L}_z

$$\begin{aligned}\vec{L} &= \vec{r} \times \vec{p} \\ &= L_x \hat{i} + L_y \hat{j} + L_z \hat{k} \\ &= (yp_z - zp_y) \hat{i} + (zp_x - xp_z) \hat{j} + (xp_y - yp_x) \hat{k} \\ &= \frac{\hbar}{i} \left[\left(y \frac{d}{dz} - z \frac{d}{dy} \right) \hat{i} + \left(z \frac{d}{dx} - x \frac{d}{dz} \right) \hat{j} + \left(x \frac{d}{dy} - y \frac{d}{dx} \right) \hat{k} \right]\end{aligned}$$

Transformation from Cartesian to spherical coordinates:

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

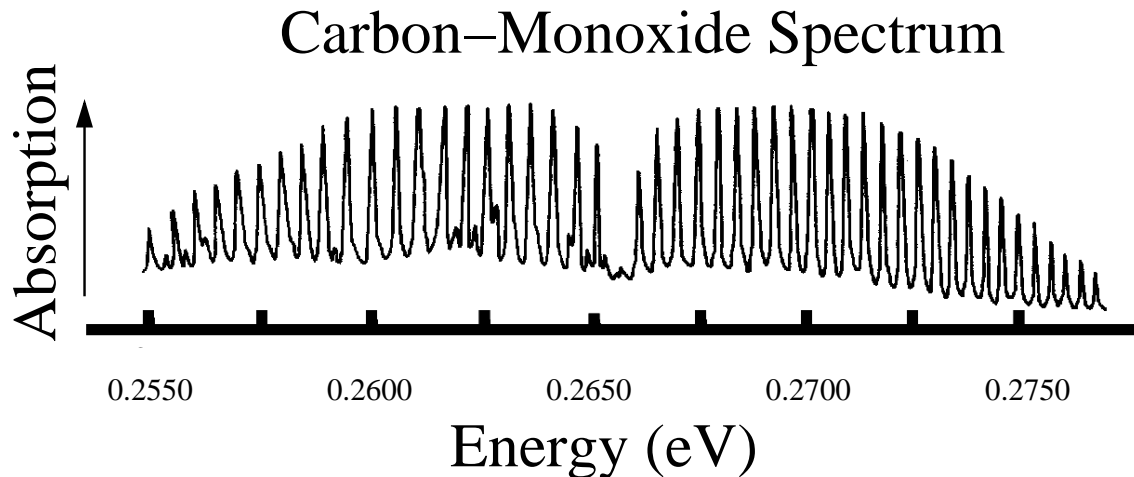


Is Carbon Monoxide A Rigid Rotator?

Excited states of carbon monoxide (CO) can be observed by passing light through a cell containing CO and measuring the absorption spectrum shown below. The molecule can both vibrate and rotate at the same time. The rotational energy states of a rigid rotator are

$$E_l = \frac{\hbar^2}{2I}l(l + 1)$$

where I is the moment of inertia. The vibrational part of the energy can be described by the harmonic oscillator so $E_n = (n + \frac{1}{2})\hbar\omega_0$ with $\Delta E = \hbar\omega_0 = 0.25 \pm 0.05 \text{ eV}$ from our previous results. How does one arrive at the expression above for the rotational energy? Is CO a rigid rotator?



Summary So Far

$$\frac{p_r^2}{2\mu} = -\frac{\hbar^2}{2\mu} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right)$$

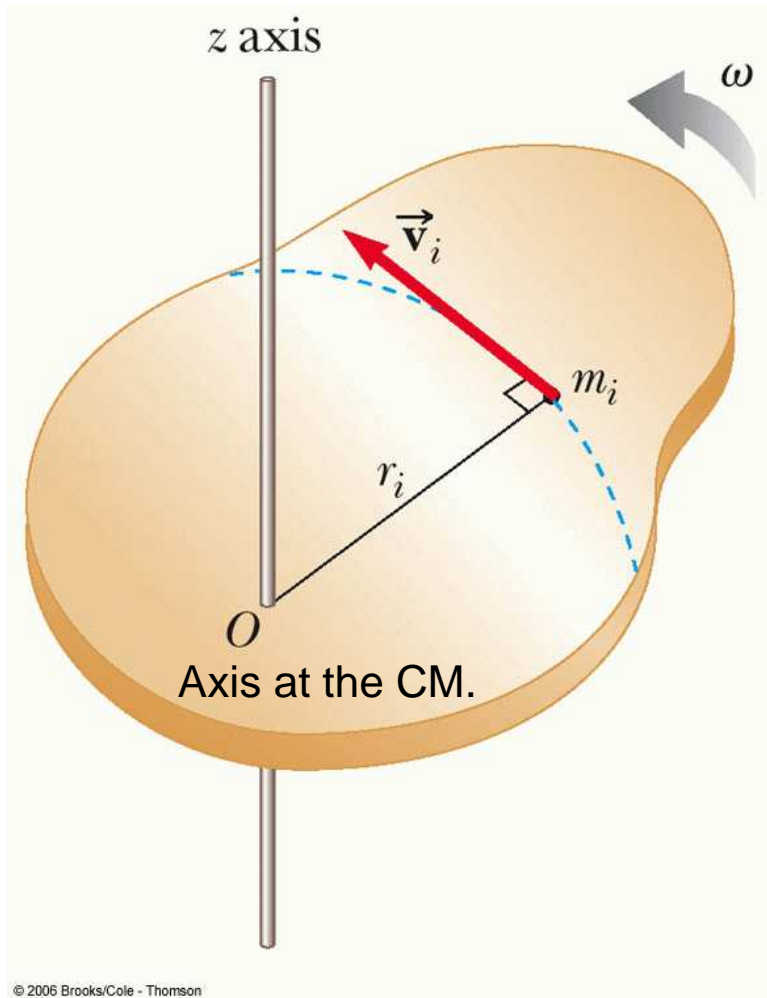
$$\frac{L^2}{2\mu r^2} = -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

$$m_l = 0, \pm \frac{1}{2}, \pm \frac{2}{2}, \pm \frac{3}{2}, \dots \quad \Phi(\phi) = \Phi_0 e^{\pm i m_l \phi}$$

$$\left[-\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{m_l^2}{\sin^2 \theta} \right] \Theta = A \Theta \quad A = l(l+1)$$

$$L^2 |\phi\rangle = \hbar^2 l(l+1) |\phi\rangle \quad L_z |\phi\rangle = \pm m_l \hbar^2 |\phi\rangle \quad \Theta(\theta) \Phi(\phi) = Y_{lm}(\theta, \phi)$$

Rotational Kinetic Energy



Rotational Kinetic Energy

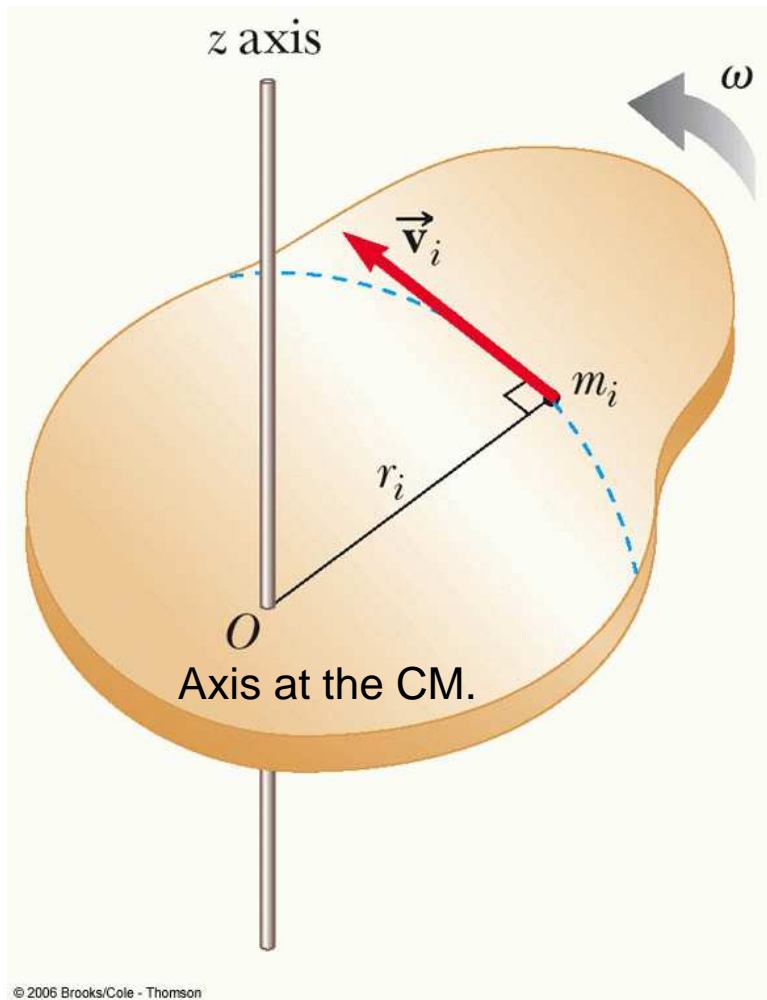
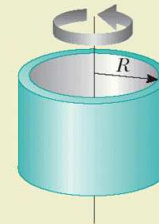
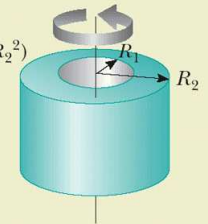


TABLE 10.2 Moments of Inertia of Homogeneous Rigid Objects With Different Geometries

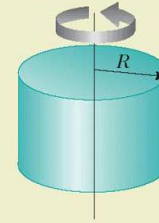
Hoop or thin cylindrical shell
 $I_{CM} = MR^2$



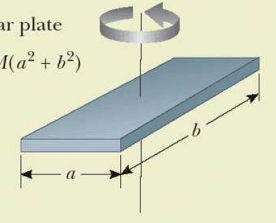
Hollow cylinder
 $I_{CM} = \frac{1}{2}M(R_1^2 + R_2^2)$



Solid cylinder or disk
 $I_{CM} = \frac{1}{2}MR^2$



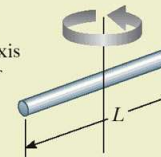
Rectangular plate
 $I_{CM} = \frac{1}{12}M(a^2 + b^2)$



© 2006 Brooks/Cole - Thomson

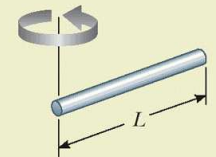
Long thin rod with rotation axis through center

$$I_{CM} = \frac{1}{12}ML^2$$

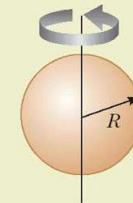


Long thin rod with rotation axis through end

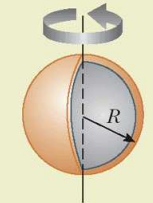
$$I = \frac{1}{3}ML^2$$



Solid sphere
 $I_{CM} = \frac{2}{5}MR^2$

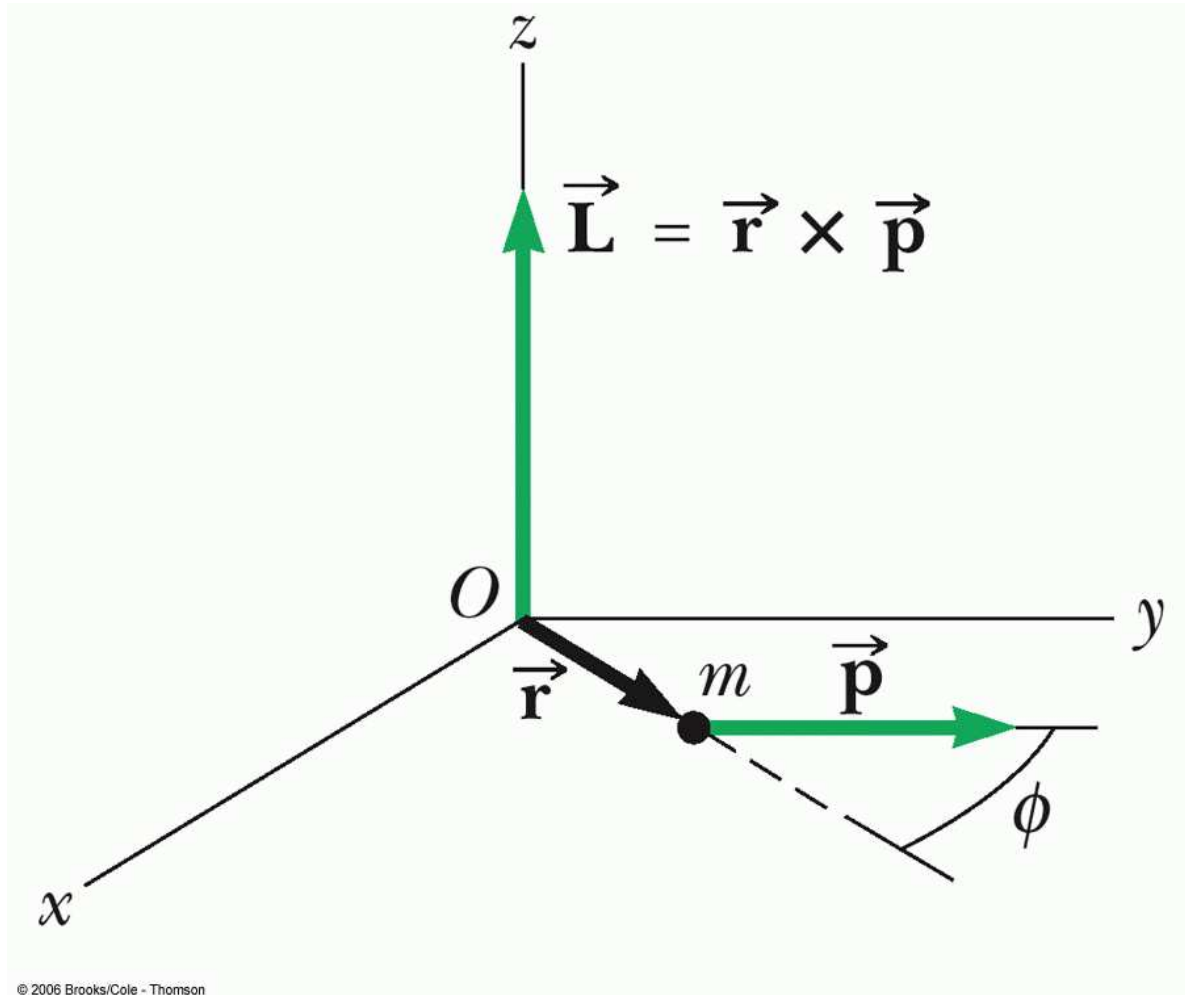


Thin spherical shell
 $I_{CM} = \frac{2}{3}MR^2$

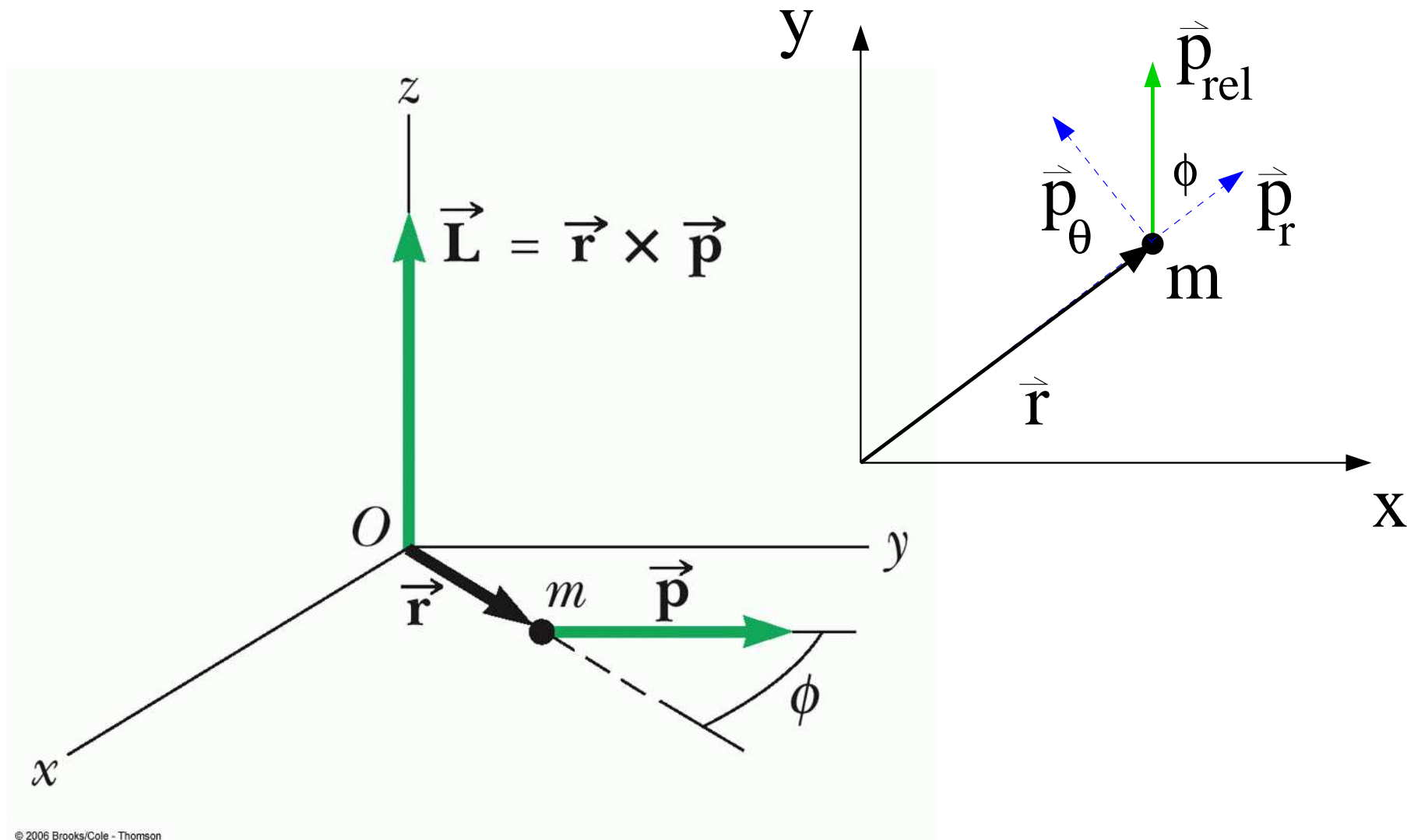


© 2006 Brooks/Cole - Thomson

Angular Momentum

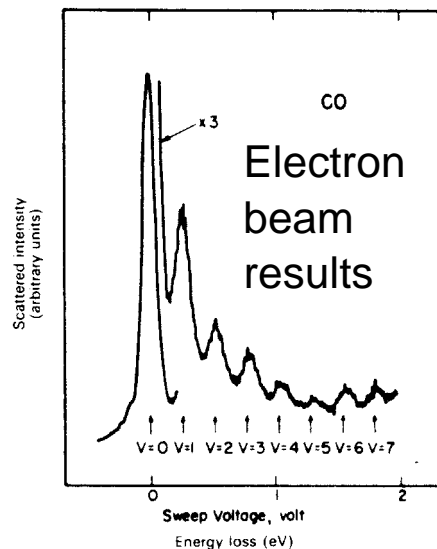


Angular Momentum



© 2006 Brooks/Cole - Thomson

Is CO a Rigid Rotator?



$$\Delta E = 0.25 \pm 0.05 \text{ eV}$$

CO Absorption Spectrum

Incident light

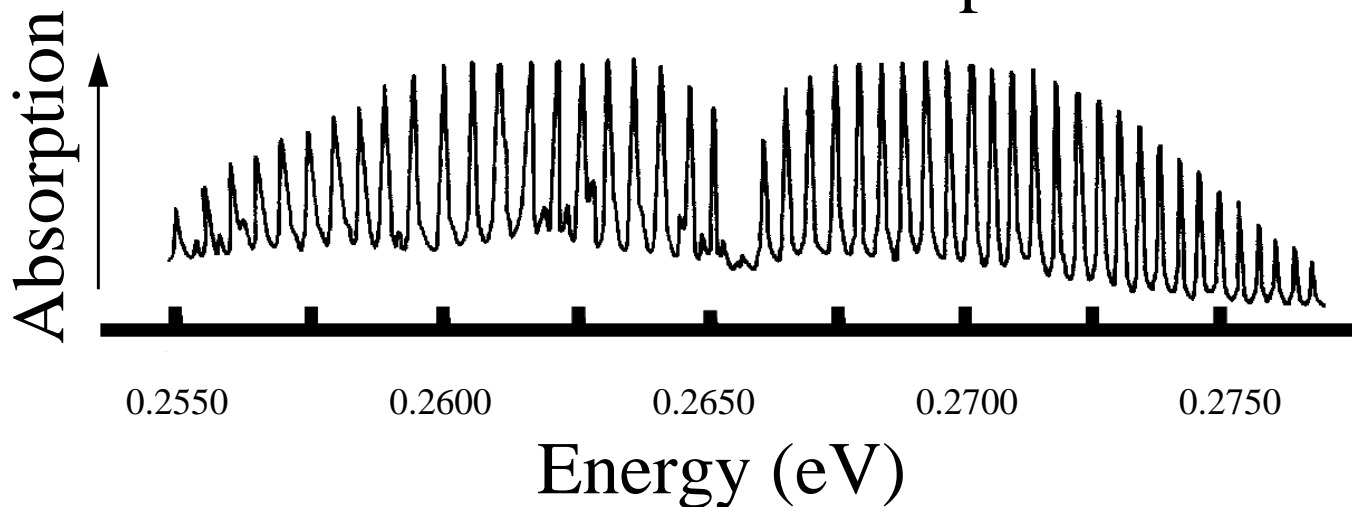


CO gas target



Photon detector

Carbon-Monoxide Spectrum



The Eigenvalues of \hat{L}^2 and \hat{L}_z

$$\begin{aligned}\vec{L} &= \vec{r} \times \vec{p} \\ &= L_x \hat{i} + L_y \hat{j} + L_z \hat{k}\end{aligned}$$

The Eigenvalues of \hat{L}^2 and \hat{L}_z

$$\vec{L} = \vec{r} \times \vec{p}$$

$$= L_x \hat{i} + L_y \hat{j} + L_z \hat{k}$$

$$= (yp_z - zp_y) \hat{i} + (zp_x - xp_z) \hat{j} + (xp_y - yp_x) \hat{k}$$

The Eigenvalues of \hat{L}^2 and \hat{L}_z

$$\begin{aligned}\vec{L} &= \vec{r} \times \vec{p} \\ &= L_x \hat{i} + L_y \hat{j} + L_z \hat{k} \\ &= (yp_z - zp_y) \hat{i} + (zp_x - xp_z) \hat{j} + (xp_y - yp_x) \hat{k} \\ &= \frac{\hbar}{i} \left[\left(y \frac{d}{dz} - z \frac{d}{dy} \right) \hat{i} + \left(z \frac{d}{dx} - x \frac{d}{dz} \right) \hat{j} + \left(x \frac{d}{dy} - y \frac{d}{dx} \right) \hat{k} \right]\end{aligned}$$

The Eigenvalues of \hat{L}^2 and \hat{L}_z

$$\begin{aligned}\vec{L} &= \vec{r} \times \vec{p} \\ &= L_x \hat{i} + L_y \hat{j} + L_z \hat{k} \\ &= (yp_z - zp_y) \hat{i} + (zp_x - xp_z) \hat{j} + (xp_y - yp_x) \hat{k} \\ &= \frac{\hbar}{i} \left[\left(y \frac{d}{dz} - z \frac{d}{dy} \right) \hat{i} + \left(z \frac{d}{dx} - x \frac{d}{dz} \right) \hat{j} + \left(x \frac{d}{dy} - y \frac{d}{dx} \right) \hat{k} \right]\end{aligned}$$

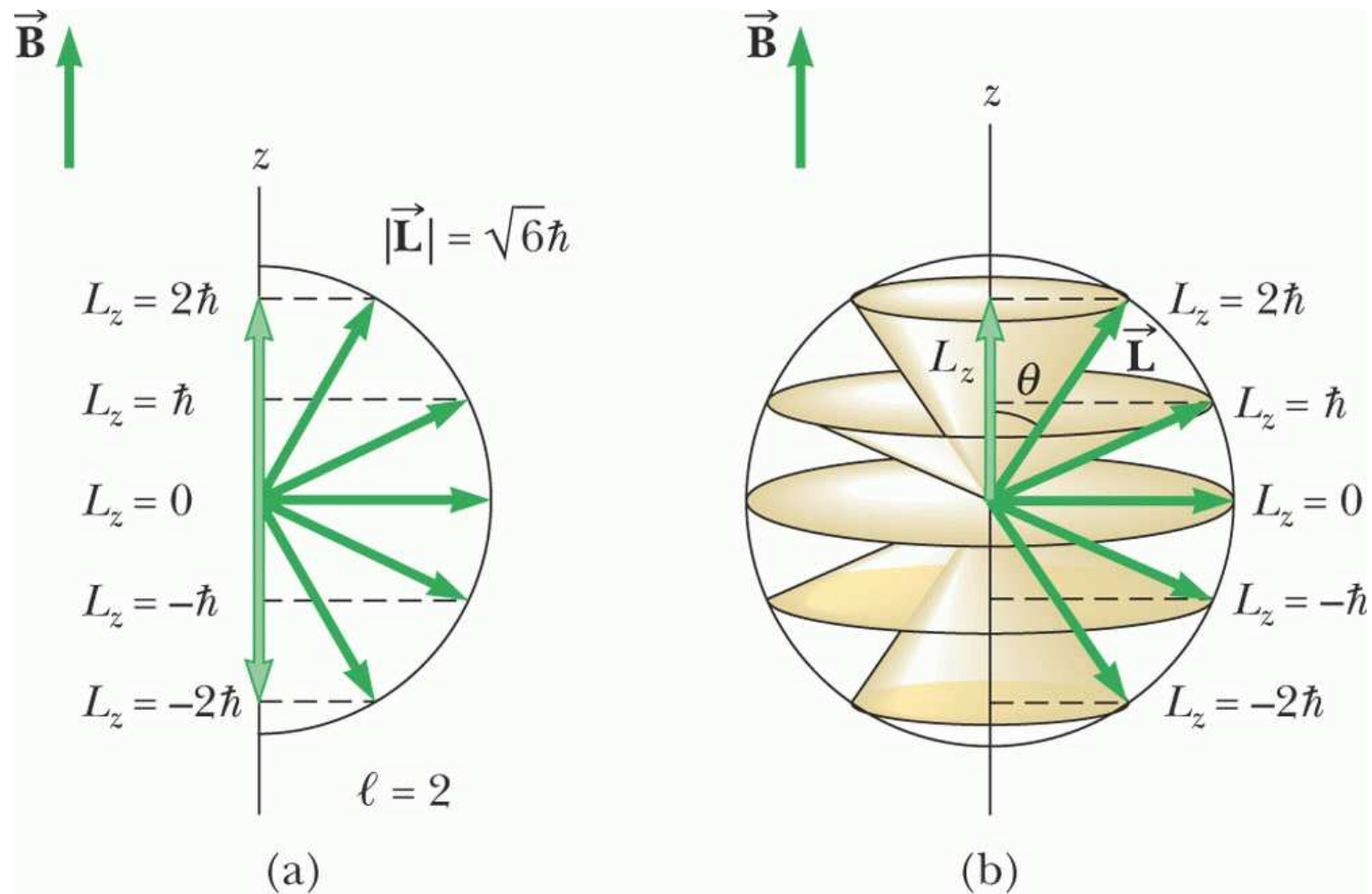
Transformation from Cartesian to spherical coordinates:

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

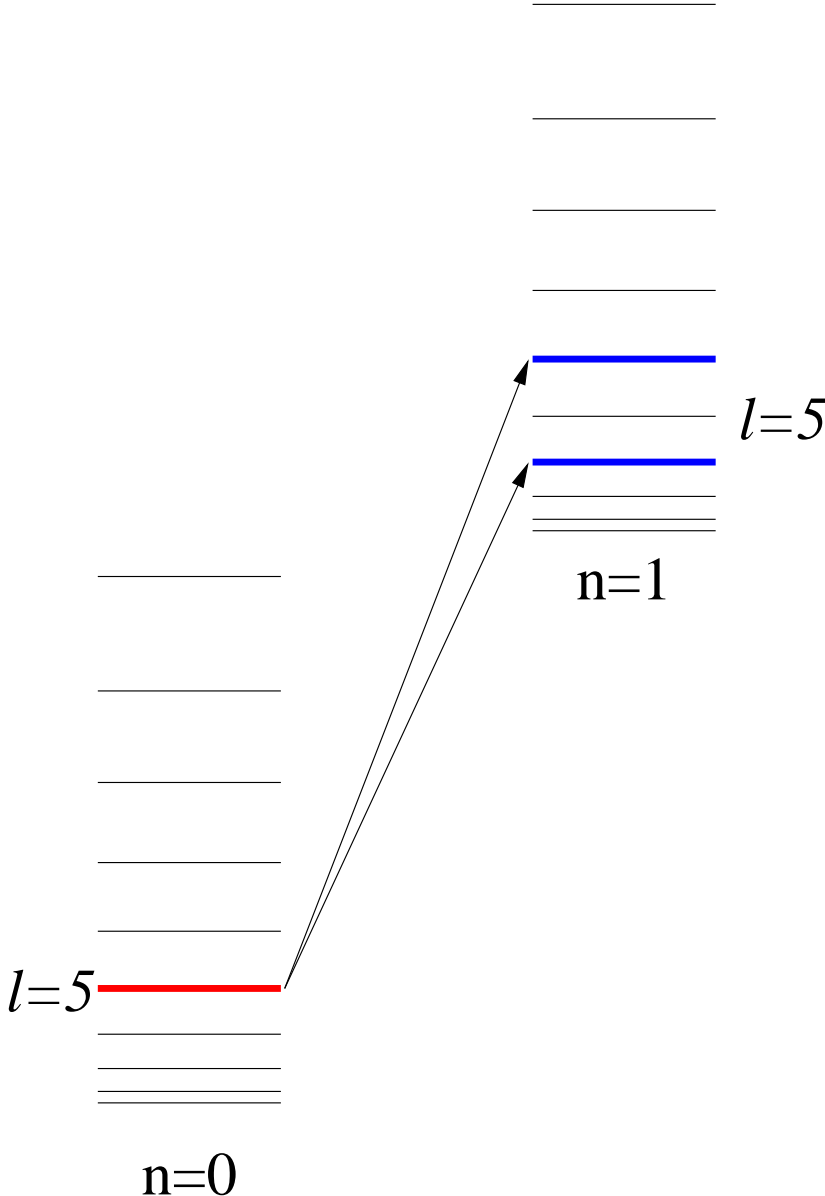
$$z = r \cos \theta$$

The Eigenvalues of \hat{L}^2 and L_z



© 2006 Brooks/Cole - Thomson

CO Atomic Transitions



Carbon Monoxide Rotation Spectrum

Rotational Spectra

