CHEM 1410 HW #5
Due Oct. 15

7.26

$\hat{L}_z p_x = -i\hbar \frac{\partial}{\partial\theta}\sqrt{\frac{3}{4\pi}} \sin\theta \cos\phi = i\hbar\sqrt{\frac{3}{4\pi}} \sin\theta \sin\phi$. This shows that p_x is not an eigenfunction of $\hat{L}_z$.

$\hat{L}_z d_{xz} = -i\hbar \frac{\partial}{\partial\theta}\sqrt{\frac{15}{4\pi}} \sin\theta \cos\theta \cos\phi = i\hbar\sqrt{\frac{15}{4\pi}} \sin\theta \cos\theta \sin\phi$. This shows that d_{xz} is not an eigenfunction of $\hat{L}_z$.

7.29

$$\frac{n_{J=1}}{n_{J=0}} = \frac{2J+1}{1} e^{-\frac{\hbar^2 J(J+1)}{2IkT}}$$

$$= 3 \exp\left[-\frac{\left(1.055\times10^{-34}\text{J s}\right)^2 1(1+1)}{2\times\frac{1.0078\times34.9688}{1.0078+34.9688}\text{amu}\times1.66\times10^{-27}\text{kg amu}^{-1}\times\left(1.27\times10^{-10}\text{m}\right)^2\times1.381\times10^{-23}\text{J K}^{-1}\times300\text{ K}}\right]$$

$$\frac{n_{J=1}}{n_{J=0}} = 2.708$$

$$\frac{n_{J=5}}{n_{J=0}} = \frac{2J+1}{1} e^{-\frac{\hbar^2 J(J+1)}{2IkT}}$$

$$= 11 \exp\left[-\frac{\left(1.055\times10^{-34}\text{J s}\right)^2 5(5+1)}{2\times\frac{1.0078\times34.9688}{1.0078+34.9688}\text{amu}\times1.66\text{x}10^{-27}\text{kg amu}^{-1}\times\left(1.27\times10^{-10}\text{m}\right)^2\times1.381\times10^{-23}\text{JK}^{-1}\times300\text{ K}}\right]$$

$$\frac{n_{J=5}}{n_{J=0}} = 2.369$$

8.4

$$E_n = h\nu\left(n+\frac{1}{2}\right) - \frac{(h\nu)^2}{4D_e}\left(n+\frac{1}{2}\right)^2 = 6.626\times10^{-34}\,\text{J s}\times 8.97\times10^{13}\text{s}^{-1}\times\left(n+\frac{1}{2}\right)$$

$$-\frac{\left(6.626\times10^{-34}\text{J s}\times8.97\times10^{13}\text{s}^{-1}\right)^2}{4\times7.41\times10^{-19}\text{J}}$$

$$E_n = 5.944\times10^{-20}\times\left(n+\frac{1}{2}\right)\text{J} - 1.192\times10^{-21}\times\left(n+\frac{1}{2}\right)^2\ \text{J}$$

$$E_0 = 2.942\times10^{-20}\ \text{J}$$

$$E_1 = 8.647\times10^{-20}\ \text{J}$$

$$E_2 = 1.411\times10^{-19}\ \text{J}$$

$$E_3 = 1.934\times10^{-19}\ \text{J}$$

$$\nu_{0\to1} = \frac{E_1 - E_0}{h} = \frac{8.647\times10^{-20}\,\text{J} - 2.942\times10^{-20}\,\text{J}}{6.626\times10^{-34}\,\text{J s}} = 8.61\times10^{13}\,\text{s}^{-1}$$

$$\nu_{0\to2} = \frac{E_1 - E_0}{h} = \frac{14.11\times10^{-20}\,\text{J} - 2.942\times10^{-20}\,\text{J}}{6.626\times10^{-34}\,\text{J s}} = 1.69\times10^{14}\,\text{s}^{-1}$$

$$\nu_{0\to3} = \frac{E_1 - E_0}{h} = \frac{19.34\times10^{-20}\,\text{J} - 2.942\times10^{-20}\,\text{J}}{6.626\times10^{-34}\,\text{J s}} = 2.47\times10^{14}\,\text{s}^{-1}$$

$$\text{Error}\left(\nu_{0\to2}\right) = \frac{\nu_{0\to2} - 2\nu_{0\to1}}{\nu_{0\to2}} = -1.89\%$$

$$\text{Error}\left(\nu_{0\to3}\right) = \frac{\nu_{0\to2} - 3\nu_{0\to1}}{\nu_{0\to2}} = -4.57\%$$

8.11

The major peak near 1700 cm^{-1} is the C=O stretch and the peak near 1200 cm^{-1} is a C–C–C stretch. These peaks are consistent with the compound being acetone. Ethyl amine should show a strong peak near 3350 cm^{-1} and pentanol should show a strong peak near 3400 cm^{-1}. Because these peaks are absent, these compounds can be ruled out.

8.15

$$B = \frac{h}{8\pi^2 \mu r_0^2}; \quad r_0 = \sqrt{\frac{h}{8\pi^2 \mu B}}$$

$$r_0 = \sqrt{\frac{6.6260755\times10^{-34}\,\mathrm{J\,s}}{8\pi^2 \times \frac{2.0141018\times18.9984032\,\mathrm{amu}}{(2.0141018+18.9984032)}\times1.6605402\times10^{-27}\,\mathrm{kg\,amu^{-1}}\times11.007\,\mathrm{cm^{-1}}\times2.99792458\times10^{10}\,\mathrm{cm\,s^{-1}}}}$$

$$r_0 = 9.1707\times10^{-11}\,\mathrm{m}$$

8.22

$$\int A_{+\phi} e^{-im_2\phi} \mu \cos\phi A_{+\phi} e^{im_1\phi} \mathrm{d}\phi = \frac{\mu\left(A_{+\phi}\right)^2}{2} \int e^{-im_2\phi}\left(e^{i\phi} + e^{-i\phi}\right) e^{im_1\phi} \mathrm{d}\phi$$

$$= \frac{\mu\left(A_{+\phi}\right)^2}{2} \int \left[e^{-i(m_2 - m_1 - 1)\phi} + e^{-i(m_2 - m_1 + 1)\phi} \right] \mathrm{d}\phi$$

This integral only has a nonzero value if one of the exponents in the integrand is zero. Therefore, $m_2 = m_1 \pm 1$.