

Problem Set 7

P19.1) The $^1\text{H}^{81}\text{Br}$ molecule can be described by a Morse potential with $D_e = 7.70 \times 10^{-19}$ J. The force constant k for this molecule is 412 N m^{-1} and $\nu = 7.94 \times 10^{13} \text{ s}^{-1}$.

a. Calculate the lowest four energy levels for a Morse potential using the formula

$$E_n = h\nu \left(n + \frac{1}{2} \right) - \frac{(h\nu)^2}{4D_e} \left(n + \frac{1}{2} \right)^2$$

b. Calculate the fundamental frequency ν_0 corresponding to the transition $n = 0 \rightarrow n = 1$ and the frequencies of the first three overtone vibrations. How large would the relative error be if you assume that the first three overtone frequencies are $2\nu_0$, $3\nu_0$, and $4\nu_0$?

$$E_n = h\nu \left(n + \frac{1}{2} \right) - \frac{(h\nu)^2}{4D_e} \left(n + \frac{1}{2} \right)^2 = 6.626 \times 10^{-34} \text{ J s} \times 7.94 \times 10^{13} \text{ s}^{-1} \times \left(n + \frac{1}{2} \right) - \frac{(6.626 \times 10^{-34} \text{ J s} \times 7.94 \times 10^{13} \text{ s}^{-1})^2}{4 \times 7.70 \times 10^{-19} \text{ J}} \left(n + \frac{1}{2} \right)^2$$

$$E_n = 5.261 \times 10^{-20} \times \left(n + \frac{1}{2} \right) \text{ J} - 8.987 \times 10^{-22} \times \left(n + \frac{1}{2} \right)^2 \text{ J}$$

$$E_0 = 2.61 \times 10^{-20} \text{ J}$$

$$E_1 = 7.69 \times 10^{-20} \text{ J}$$

$$E_2 = 1.26 \times 10^{-19} \text{ J}$$

$$E_3 = 1.73 \times 10^{-19} \text{ J}$$

$$\nu_{0 \rightarrow 1} = \frac{E_1 - E_0}{h} = \frac{7.69 \times 10^{-20} \text{ J} - 2.61 \times 10^{-20} \text{ J}}{6.626 \times 10^{-34} \text{ J s}} = 7.67 \times 10^{13} \text{ s}^{-1}$$

$$\nu_{0 \rightarrow 2} = \frac{E_2 - E_0}{h} = \frac{12.6 \times 10^{-20} \text{ J} - 2.61 \times 10^{-20} \text{ J}}{6.626 \times 10^{-34} \text{ J s}} = 1.51 \times 10^{14} \text{ s}^{-1}$$

$$\nu_{0 \rightarrow 3} = \frac{E_3 - E_0}{h} = \frac{17.3 \times 10^{-20} \text{ J} - 2.61 \times 10^{-20} \text{ J}}{6.626 \times 10^{-34} \text{ J s}} = 2.22 \times 10^{14} \text{ s}^{-1}$$

$$\text{Error}(\nu_{0 \rightarrow 2}) = \frac{\nu_{0 \rightarrow 2} - 2\nu_{0 \rightarrow 1}}{\nu_{0 \rightarrow 2}} = -1.8\%$$

$$\text{Error}(\nu_{0 \rightarrow 3}) = \frac{\nu_{0 \rightarrow 3} - 3\nu_{0 \rightarrow 1}}{\nu_{0 \rightarrow 3}} = -3.7\%$$

P19.13) Selection rules in the dipole approximation are determined by the integral $\mu_x^{mn} = \int \psi_m^*(x) \mu_x(x) \psi_n(x) dx$. If this integral is nonzero, the transition will be observed in an absorption spectrum. If the integral is zero, the transition is “forbidden” in the dipole approximation. It actually occurs with low probability because the dipole approximation is not exact. Consider the particle in the one-dimensional box and set $\mu_x = -ex$.

a. Calculate μ_x^{12} and μ_x^{13} in the dipole approximation. Can you see a pattern and discern a selection rule?

You may need to evaluate a few more integrals of the type μ_x^{lm} . The standard integral

$$\int x \sin \frac{\pi x}{a} \sin \frac{n\pi x}{a} dx = \frac{1}{2} \left(\frac{a^2 \cos \frac{(n-1)\pi x}{a}}{(n-1)^2 \pi^2} + \frac{a x \sin \frac{(n-1)\pi x}{a}}{(n-1)\pi} \right) - \frac{1}{2} \left(\frac{a^2 \cos \frac{(n+1)\pi x}{a}}{(n+1)^2 \pi^2} + \frac{a x \sin \frac{(n+1)\pi x}{a}}{(n+1)\pi} \right)$$

is useful for solving this problem.

b. Determine the ratio μ_x^{12}/μ_x^{14} . On the basis of your result, would you modify the selection rule that you determined in part a?

a) We first evaluate μ_x^{12} .

$$\begin{aligned} \mu_x^{12} &= -\frac{2e}{a} \int_0^a x \sin \frac{\pi x}{a} \sin \frac{2\pi x}{a} dx = \left[-\frac{e}{a} \left(\frac{a^2 \cos \frac{\pi x}{a}}{\pi^2} + \frac{a x \sin \frac{\pi x}{a}}{\pi} \right) \right. \\ &\quad \left. + \frac{e}{a} \left(\frac{a^2 \cos \frac{3\pi x}{a}}{9\pi^2} + \frac{3a x \sin \frac{3\pi x}{a}}{9\pi} \right) \right]_0^a \\ &= -\frac{e}{a} \left(\frac{a^2 \cos \pi}{\pi^2} + \frac{a \sin \pi}{\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos 3\pi}{9\pi^2} + \frac{a \sin 3\pi}{3\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos 0}{\pi^2} + 0 \right) - \frac{e}{a} \left(\frac{a^2 \cos 0}{9\pi^2} - 0 \right) \text{ The result is} \\ &= -\frac{e}{a} \left(-\frac{a^2}{\pi^2} + 0 \right) - \frac{e}{a} \left(\frac{a^2}{9\pi^2} + 0 \right) + \frac{e}{a} \left(\frac{a^2}{\pi^2} + 0 \right) - \frac{e}{a} \left(\frac{a^2}{9\pi^2} + 0 \right) = 2 \frac{ea}{\pi^2} - \frac{2ea}{9\pi^2} = \frac{16ea}{9\pi^2} \\ \mu_x^{12} &= \frac{2e}{a} \frac{8a^2}{9\pi^2} = \frac{16ae}{9\pi^2} \end{aligned}$$

$$\begin{aligned}
\mu_x^{13} &= -\frac{2e}{a} \int_0^a x \sin \frac{\pi x}{a} \sin \frac{3\pi x}{a} dx \\
&= \left[-\frac{e}{a} \left(\frac{a^2 \cos \frac{2\pi x}{a}}{4\pi^2} + \frac{2ax \sin \frac{2\pi x}{a}}{4\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos \frac{4\pi x}{a}}{16\pi^2} + \frac{4ax \sin \frac{4\pi x}{a}}{16\pi} \right) \right]_0^a \\
&= -\frac{e}{a} \left(\frac{a^2 \cos 2\pi}{4\pi^2} + \frac{2a^2 \sin 2\pi}{4\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos 4\pi}{16\pi^2} + \frac{4a^2 \sin \frac{4\pi x}{a}}{16\pi} \right) \\
&\quad + \frac{e}{a} \left(\frac{a^2 \cos 0}{4\pi^2} + 0 \right) - \frac{e}{a} \left(\frac{a^2 \cos 0}{16\pi^2} + 0 \right) \\
&= -\frac{e}{a} \left(\frac{a^2}{4\pi^2} + 0 \right) + \frac{e}{a} \left(\frac{a^2}{16\pi^2} + 0 \right) + \frac{e}{a} \left(\frac{a^2}{4\pi^2} + 0 \right) - \frac{e}{a} \left(\frac{a^2}{16\pi^2} + 0 \right) = 0
\end{aligned}$$

The result is $\mu_x^{13} = 0$.

$$\begin{aligned}
\mu_x^{14} &= -\frac{2e}{a} \int_0^a x \sin \frac{\pi x}{a} \sin \frac{4\pi x}{a} dx \\
&= \left[-\frac{e}{a} \left(\frac{a^2 \cos \frac{3\pi x}{a}}{9\pi^2} + \frac{3ax \sin \frac{3\pi x}{a}}{9\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos \frac{5\pi x}{a}}{25\pi^2} + \frac{5ax \sin \frac{5\pi x}{a}}{25\pi} \right) \right]_0^a \\
&= -\frac{e}{a} \left(\frac{a^2 \cos 3\pi}{9\pi^2} + \frac{3a^2 \sin 3\pi}{9\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos 5\pi}{25\pi^2} + \frac{5a^2 \sin 5\pi}{25\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos 0}{9\pi^2} + 0 \right) \\
&\quad - \frac{e}{a} \left(\frac{a^2 \cos 0}{25\pi^2} + 0 \right) \\
&= -\frac{e}{a} \left(-\frac{a^2}{9\pi^2} + 0 \right) + \frac{e}{a} \left(-\frac{a^2}{25\pi^2} + 0 \right) + \frac{e}{a} \left(\frac{a^2}{9\pi^2} + 0 \right) - \frac{e}{a} \left(\frac{a^2}{25\pi^2} + 0 \right) = \frac{2ea}{9\pi^2} - \frac{2ea}{25\pi^2} \\
&= \frac{32ea}{225\pi^2}
\end{aligned}$$

The result is $\mu_x^{14} = \frac{32ea}{225\pi^2}$.

$$\begin{aligned}
\mu_x^{15} &= -\frac{2e}{a} \int_0^a x \sin \frac{\pi x}{a} \sin \frac{5\pi x}{a} dx \\
&= \left[-\frac{e}{a} \left(\frac{a^2 \cos \frac{4\pi x}{a}}{16\pi^2} + \frac{4ax \sin \frac{4\pi x}{a}}{16\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos \frac{6\pi x}{a}}{36\pi^2} + \frac{6ax \sin \frac{6\pi x}{a}}{36\pi} \right) \right]_0^a \\
&= -\frac{e}{a} \left(\frac{a^2 \cos 4\pi}{16\pi^2} + \frac{4a^2 \sin 4\pi}{16\pi} \right) + \frac{e}{a} \left(\frac{a^2 \cos 6\pi}{36\pi^2} + \frac{6a^2 \sin \frac{6\pi x}{a}}{36\pi} \right) \\
&\quad + \frac{e}{a} \left(\frac{a^2 \cos 0}{16\pi^2} + 0 \right) - \frac{e}{a} \left(\frac{a^2 \cos 0}{36\pi^2} + 0 \right) \\
&= -\frac{e}{a} \left(\frac{a^2}{16\pi^2} + 0 \right) + \frac{e}{a} \left(\frac{a^2}{36\pi^2} + 0 \right) + \frac{e}{a} \left(\frac{a^2}{16\pi^2} + 0 \right) - \frac{e}{a} \left(\frac{a^2}{36\pi^2} + 0 \right) = 0
\end{aligned}$$

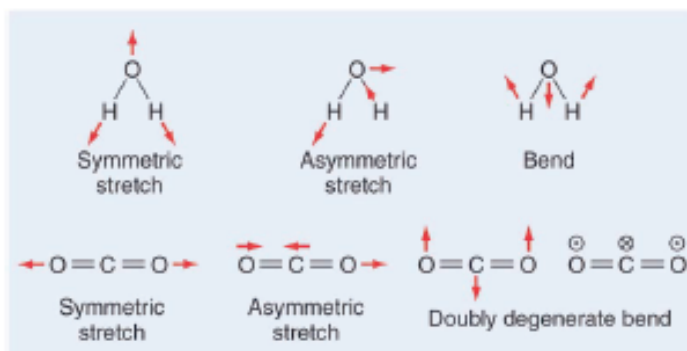
The result is $\mu_x^{15} = 0$.

These results show that the $1 \rightarrow n$ transition is allowed only if n is even, or that the initial and final states have opposite parity with respect to reflection about the center of the box.

b) $\mu_x^{12}/\mu_x^{14} = \left(\frac{16ae}{9\pi^2} \right) / \left(\frac{32ea}{225\pi^2} \right) = 12.5$. It turns out that $\mu_x^{12}/\mu_x^{16} = 45.4$. This means that the transitions

from $n = 1$ to $n = 4$ and 6 are much weaker than the transition from $n = 1$ to 2 . Therefore, effectively, the selection rule is $\Delta n = 1$ for absorption.

P19.15) Calculating the motion of individual atoms in the vibrational modes of molecules (called normal modes) is an advanced topic. Given the normal modes shown in the following figure, decide which of the normal modes of CO_2 and H_2O have a nonzero dynamical dipole moment and are therefore infrared active. The motion of the atoms in the second of the two doubly degenerate bend modes for CO_2 is identical to the first, but is perpendicular to the plane of the page.



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All three vibrational modes of water will lead to a change in the dipole moment and are therefore infrared active. The symmetric stretch of carbon dioxide will not lead to a change in the dipole moment and is infrared inactive. The other two modes will lead to a change in the dipole moment and are infrared active.

P19.17) The rigid rotor model can be improved by recognizing that in a realistic anharmonic potential, the bond length increases with the vibrational quantum number n . Therefore, the rotational constant depends on n , and it can be shown that $B_n = B - (n + 1/2)\alpha$, where B is the rigid rotor value. The constant α can be obtained from experimental spectra. For $^1\text{H}^{127}\text{I}$, $B = 6.551 \text{ cm}^{-1}$ and $\alpha = 0.183 \text{ cm}^{-1}$. Using this more accurate formula for B_n , calculate the bond length for HI in the ground state and for $n = 3$.

For $n = 0$

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

$$r_0 = \sqrt{\frac{6.6260755 \times 10^{-34} \text{ J s}}{8\pi^2 \times \frac{1.0078250 \text{ amu} \times 126.9045 \text{ amu}}{1.0078250 \text{ amu} + 126.9045 \text{ amu}} \times 1.6605402 \times 10^{-27} \text{ kg amu}^{-1} \times \left(6.551 - \frac{0.183}{2}\right) \text{ cm}^{-1} \times 2.99792458 \times 10^{10} \text{ cm s}^{-1}}}$$

$$r_0 = 1.62 \times 10^{-10} \text{ m}$$

For $n = 3$

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

$$r_0 = \sqrt{\frac{6.6260755 \times 10^{-34} \text{ J s}}{8\pi^2 \times \frac{1.0078250 \text{ amu} \times 126.9045 \text{ amu}}{1.0078250 \text{ amu} + 126.9045 \text{ amu}} \times 1.6605402 \times 10^{-27} \text{ kg amu}^{-1} \times \left(6.551 - \frac{3 \times 0.183}{2}\right) \text{ cm}^{-1} \times 2.99792458 \times 10^{10} \text{ cm s}^{-1}}}$$

$$r_0 = 1.69 \times 10^{-10} \text{ m}$$

P19.18) Greenhouse gases generated from human activity absorb infrared radiation from the Earth and keep it from being dispersed outside our atmosphere. This is a major cause of global warming. Compare the path length required to absorb 90.% of the Earth's radiation near a wavelength of $7 \mu\text{m}$ for CH_3CCl_3 [$\epsilon(\lambda) = 1.8 \text{ (cm atm)}^{-1}$] and the chlorofluorocarbon CFC-14 [$\epsilon(\lambda) = 4.1 \times 10^3 \text{ (cm atm)}^{-1}$] assuming that each of these gases has a partial pressure of 2.0×10^{-6} bar and that the total pressure is 1 bar.

Rearranging the Beer-Lambert equation, we have for CH_3CCl_3

$$l = -\frac{1}{M\epsilon(\lambda)} \ln\left(\frac{I(\lambda)}{I_0(\lambda)}\right) = -\frac{1}{1.8 \text{ (cm atm)}^{-1} \times 2.0 \times 10^{-6} \text{ atm}} \times \ln 0.10 = 6.1 \times 10^5 \text{ cm}$$

For CFC-14 we have

$$l = -\frac{1}{M\epsilon(\lambda)} \ln\left(\frac{I(\lambda)}{I_0(\lambda)}\right) = -\frac{1}{4.1 \times 10^3 \text{ (cm atm)}^{-1} \times 2.0 \times 10^{-6} \text{ atm}} \times \ln 0.10 = 2.7 \times 10^2 \text{ cm}$$

P19.22) Overtone transitions in vibrational absorption spectra for which $\Delta n = +2, +3, \dots$ are forbidden for the harmonic potential $V = (1/2)kx^2$ because $\mu_x^{mn} = 0$ for $|m-n| \neq 1$ as shown in Section 19.4. However, overtone transitions are allowed for the more realistic anharmonic potential. In this problem, you will explore how the selection rule is modified by including anharmonic terms in the potential. We do so in an indirect manner by including additional terms in the expansion of the dipole moment $\mu_x(x) = \mu_{0x} + x (d\mu_x/dx)_e + \dots$, but assuming that the harmonic oscillator total energy eigenfunctions are still valid. This approximation is valid if the anharmonic correction to the harmonic potential is

$$\Delta V \ll$$

small. You will show that including the next term in the expansion of the dipole moment, which is proportional to x^2 , makes the transitions $\Delta n = \pm 2$ allowed.

a. Show that Equation (19.8) becomes

$$\begin{aligned} \mu_x^{m0} &= A_m A_0 \mu_{0x} \int_{-\infty}^{\infty} H_m(\alpha^{1/2}x) H_0(\alpha^{1/2}x) e^{-\alpha x^2} dx \\ &+ A_m A_0 \left(\frac{d\mu_x}{dx}\right)_{x=0} \int_{-\infty}^{\infty} H_m(\alpha^{1/2}x) x H_0(\alpha^{1/2}x) e^{-\alpha x^2} dx \\ &+ \frac{A_m A_0}{2!} \left(\frac{d^2\mu_x}{dx^2}\right)_{x=0} \int_{-\infty}^{\infty} H_m(\alpha^{1/2}x) x^2 H_0(\alpha^{1/2}x) e^{-\alpha x^2} dx \end{aligned}$$

b. Evaluate the effect of adding the additional term to μ_x^m . You will need the recursion relationship

$$\alpha^{1/2} x H_n(\alpha^{1/2} x) = n H_{n-1}(\alpha^{1/2} x) + \frac{1}{2} H_{n+1}(\alpha^{1/2} x).$$

Show that both the transitions $n = 0 \rightarrow n = 1$ and $n = 0 \rightarrow n = 2$ are allowed in this case.

$$\begin{aligned} x^2 H_n(\alpha^{1/2} x) &= x(x H_n(\alpha^{1/2} x)) = n \alpha^{-1/2} x H_{n-1}(\alpha^{1/2} x) + \frac{1}{2} \alpha^{-1/2} x H_{n+1}(\alpha^{1/2} x) \\ &= n \alpha^{-1/2} \left\{ (n-1) \alpha^{-1/2} H_{n-2}(\alpha^{1/2} x) + \frac{1}{2} \alpha^{-1/2} H_n(\alpha^{1/2} x) \right\} \\ &\quad + \frac{1}{2} \alpha^{-1/2} \left\{ (n+1) \alpha^{-1/2} H_n(\alpha^{1/2} x) + \frac{1}{2} \alpha^{-1/2} H_{n+2}(\alpha^{1/2} x) \right\} \\ &= \frac{n(n-1)}{\alpha} H_{n-2}(\alpha^{1/2} x) + \frac{2n+1}{2\alpha} H_n(\alpha^{1/2} x) + \frac{1}{4\alpha} H_{n+2}(\alpha^{1/2} x) \end{aligned}$$

After substitution of the above result into the integral $\int_{-\infty}^{\infty} H_m(\alpha^{1/2} x) x^2 H_n(\alpha^{1/2} x) e^{-ax^2} dx$, the integrals

$$\int_{-\infty}^{\infty} H_m(\alpha^{1/2} x) H_{n-2}(\alpha^{1/2} x) e^{-ax^2} dx, \quad \int_{-\infty}^{\infty} H_m(\alpha^{1/2} x) H_n(\alpha^{1/2} x) e^{-ax^2} dx, \quad \text{and}$$

$$\int_{-\infty}^{\infty} H_m(\alpha^{1/2} x) H_{n+2}(\alpha^{1/2} x) e^{-ax^2} dx \text{ will arise. Because of the orthogonality of the Hermite polynomials,}$$

the second integral is zero for $m \neq n$. The first and third integrals are nonzero only if $m = n + 2$ or $m = n - 2$. This result shows that additional peaks corresponding to $\Delta n = \pm 2$, corresponding to the first overtone, will appear in the vibrational spectrum due to the additional term in μ_x^m .

P19.25) Isotopic substitution is used to identify characteristic groups in an unknown compound using vibrational spectroscopy. Consider the C=C bond in ethene ($^{12}\text{C}_2\text{H}_4$). By what factor would the frequency change if deuterium were substituted for all the hydrogen atoms? Treat the H and D atoms as being rigidly attached to the carbon.

$$\frac{\nu_{\text{D}}}{\nu_{\text{H}}} = \sqrt{\frac{\mu_{\text{CH}_2\text{-CH}_2}}{\mu_{\text{CD}_2\text{-CD}_2}}} = \sqrt{\frac{\frac{(14.0156)^2}{28.0312} \text{ amu}}{\frac{(16.028)^2}{32.056} \text{ amu}}} = 0.935$$

P19.29 Because the intensity of a transition to first order is proportional to the population of the originating state, the J value for which the maximum intensity is observed in a rotational-vibrational spectrum is not generally $J=0$. Treat J in the equation

$$\frac{n_J}{n_0} = \frac{g_J}{g_0} e^{-(e_J - e_0)/kT} = (2J+1) e^{-h^2 J(J+1)/2IkT}$$

as a continuous variable.

a. Show that

$$\frac{d\left(\frac{n_J}{n_0}\right)}{dJ} = 2e^{-h^2 J(J+1)/2IkT} - \frac{(2J+1)^2 h^2}{2IkT} e^{-h^2 J(J+1)/2IkT}$$

b. Show that setting $d(n_J/n_0)/dJ = 0$ gives the equation

$$2 - \frac{(2J_{\max} + 1)^2 h^2}{2IkT} = 0$$

c. Show that the solution of this quadratic equation is

$$J_{\max} = \frac{1}{2} \left[\sqrt{\frac{4IkT}{h^2}} - 1 \right]$$

In this problem, we assume that the intensity of the individual peaks is solely determined by the population in the originating state and that it does not depend on the initial and final J values.

$$2 - \frac{(2J+1)^2 h^2}{2IkT} = 0; \quad -\frac{2h^2}{IkT} J^2 - \frac{2h^2}{IkT} J - \frac{2h^2}{IkT} + 2 = 0$$

$$\text{Solving this quadratic equation, } J_{\max} = -\frac{1}{2} \pm \frac{\sqrt{2}}{2} \sqrt{\frac{2IkT}{h^2}}$$

Only the + solution gives $J > 0$

$$J_{\max} = \frac{1}{2} \left[\sqrt{\frac{4IkT}{h^2}} - 1 \right]$$

P19.35) A measurement of the vibrational energy levels of $^{12}\text{C}^{16}\text{O}$ gives the relationship

$$\nu(n) = 2170.21\left(n + \frac{1}{2}\right) \text{ cm}^{-1} - 13.461\left(n + \frac{1}{2}\right)^2 \text{ cm}^{-1}$$

where n is the vibrational quantum number. The fundamental vibrational frequency is

$\tilde{\nu}_0 = 2170.21 \text{ cm}^{-1}$. From these data, calculate the depth D_e of the Morse potential for $^{12}\text{C}^{16}\text{O}$. Calculate the bond energy of the molecule.

We convert the expression to one in terms of energy

$$E(n) = 2170.21 \times hc \left(n + \frac{1}{2}\right) - 13.461 \times hc \left(n + \frac{1}{2}\right)^2$$

and compare it with Equation (19.5) for the Morse potential.

$$E_n = h\nu \left(n + \frac{1}{2}\right) - \frac{(h\nu)^2}{4D_e} \left(n + \frac{1}{2}\right)^2$$

from which we see that

$$13.461 \times hc = \frac{(h\nu)^2}{4D_e}$$

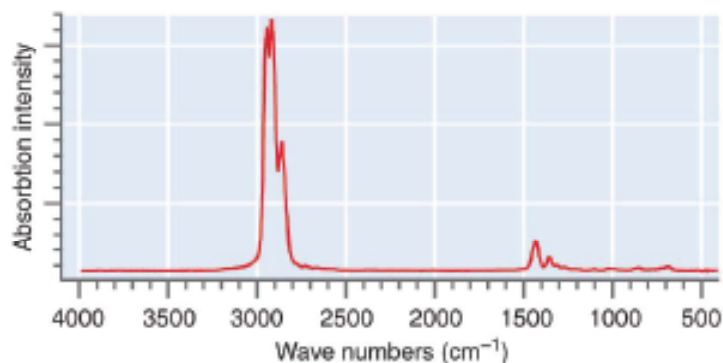
$$D_e = \frac{h\nu^2}{4 \times 13.461 \times c} = \frac{hc\tilde{\nu}^2}{4 \times 13.461}$$

$$= \frac{6.626 \times 10^{-34} \text{ J s} \times 2.998 \times 10^{10} \text{ cm s}^{-1} \times (2170 \text{ cm}^{-1})^2}{4 \times 13.461} = 1.738 \times 10^{-18} \text{ J}$$

$$D_0 = D_e - \frac{1}{2}hc\tilde{\nu}_0 = 1.738 \times 10^{-18} \text{ J} - \frac{1}{2} \times 6.626 \times 10^{-34} \text{ J s} \times 2.998 \times 10^{10} \text{ cm s}^{-1} \times 2170 \text{ cm}^{-1} \\ = 1.717 \times 10^{-18} \text{ J}$$

The bond energy per mole is $D_0 N_A = 1.034 \times 10^3 \text{ kJ mol}^{-1}$.

P19.41) An infrared absorption spectrum of an organic compound is shown in the following figure. Use the characteristic group frequencies listed in Section 19.5 to decide whether this compound is more likely to be hexene, hexane, or hexanol.



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The group of peaks near 2900 cm^{-1} is due to CH_3 and CH_2 stretching vibrations and the small peak near 1400 cm^{-1} is due to a CH_3 umbrella bending mode. These peaks are consistent with the compound being hexane. Hexene should show a strong peak near 1650 cm^{-1} and hexanol should show a strong peak near 3400 cm^{-1} . Because these peaks are absent, these compounds can be ruled out.