Chapter 2

Quantum Mechanics and Spectroscopy

Problem 2.1: Calculate the wavelength and energy of photons necessary to promote an electron from the n = 3 state to the n = 4, 5, 6, and 7 states in hydrogen. Label the region of the electromagnetic spectrum for each of the emission lines.

$$\Delta E = E_{photon} = -2.179 \ x \ 10^{-18} \ J \ \left(Z^2\right)\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \qquad \text{Eq. 2.6}$$

For n=3 → n=4 : $E_{photon} = \left[-2.179 \ x \ 10^{-18} \ J \ \left(1^2\right)\left(\frac{1}{4^2} - \frac{1}{3^2}\right)\right]$ = **1.05$\underline{9}$2 x 10^{-19} J**

From Eq. 2.4:

$$E_{photon} = \frac{hc}{\lambda} \quad \text{so} \quad \lambda = \frac{hc}{E} = \frac{\left(6.626 \ x \ 10^{-34} \ J \cdot s\right)\left(2.998 \ x \ 10^{8} \ m/s\right)}{1.0592 \ x \ 10^{-19} \ j}$$ = **1.87$\underline{5}$4 x 10^{-}**

^{6} m or 1875 nm

this is in the Near IR

For n=3 → n=5 : $E_{photon} = \left[-2.179 \ x \ 10^{-18} \ J \ \left(1^2\right)\left(\frac{1}{3^2} - \frac{1}{5^2}\right)\right]$ = **1.54$\underline{9}$5 x 10^{-19} J**

$$E_{photon} = \frac{hc}{\lambda} \quad \text{so} \quad \lambda = \frac{hc}{E} = \frac{\left(6.626 \ x \ 10^{-34} \ J \cdot s\right)\left(2.998 \ x \ 10^{8} \ m/s\right)}{1.5495 \ x \ 10^{-19} \ j}$$ = **1.28$\underline{2}$0 x 10^{-}**

^{6} m or 1282 nm

this is in the Near IR

For n=3 → n=6 : $E_{photon} = \left[-2.179 \ x \ 10^{-18} \ J \ \left(1^2\right)\left(\frac{1}{3^2} - \frac{1}{6^2}\right)\right]$ = **1.81$\underline{5}$8 x 10^{-19} J**

$$E_{photon} = \frac{hc}{\lambda} \quad \text{so} \quad \lambda = \frac{hc}{E} = \frac{\left(6.626 \ x \ 10^{-34} \ J \cdot s\right)\left(2.998 \ x \ 10^{8} \ m/s\right)}{1.8158 \ x \ 10^{-19} \ j}$$ = **1.09$\underline{4}$0 x 10^{-}**

^{6} m or 1094 nm

this is in the Near IR

For n=3 → n=7 : $E_{photon} = \left[-2.179 \ x \ 10^{-18} \ J \ \left(1^2\right)\left(\frac{1}{3^2} - \frac{1}{4^2}\right)\right]$ = **1.97$\underline{6}$4 x 10^{-19} J**

$$E_{photon} = \frac{hc}{\lambda} \quad \text{so} \quad \lambda = \frac{hc}{E} = \frac{\left(6.626 \ x \ 10^{-34} \ J \cdot s\right)\left(2.998 \ x \ 10^{8} \ m/s\right)}{1.9764 \ x \ 10^{-19} \ j}$$ = **1.00$\underline{5}$1 x 10^{-}**

^{6} m or 1005 nm

this is in the Near IR

Problem 2.2: Can an electron in a hydrogen atom moving from one energy level to a lower energy level cause a transition in the microwave region of the spectrum? Investigate only transitions between adjacent states of principal quantum number n.

We know that as n → ∞, Δn → 0. So the largest energy difference will be from n=1 → n=2.

For n=2 → n=1 : $E_{photon} = \left[-2.179 \;x\; 10^{-18} \;J\; (1^2)\left(\frac{1}{1^2} - \frac{1}{2^2}\right)\right]$ = **$-1.6342 \;x\; 10^{-18}$ J**

The negative sign here indicates that this is an exothermic process (emission of a photon as the electron drops from n=2 to n=1.

$E_{photon} = \frac{hc}{\lambda}$ so $\lambda = \frac{hc}{E} = \frac{(6.626 \;x\; 10^{-34} \;J \cdot s)(2.998 \;x\; 10^{8} \;m/s)}{1.6342 \;x\; 10^{-18} \;j}$ = **$1.216 \;x\; 10^{-7}$ m or 122 nm**

this is in the UV

So on the “bottom” end of energy levels, we know that the transitions are not near the microwave (see Problem 2.1).

We know of only 7 main energy levels in any atom, so let’s err on the side of caution and investigate a transition between energy levels twice that high, between a theoretical n=14 to n=13. If that energy level difference is higher in energy than the microwave region, we can safely assume that no transitions within the H-atom will happen in the microwave region.

For n=14 → n=13 : $E_{photon} = \left[-2.179 \;x\; 10^{-18} \;J\; (1^2)\left(\frac{1}{13^2} - \frac{1}{14^2}\right)\right]$ = **$1.776 \;x\; 10^{-21}$ J**

$E_{photon} = \frac{hc}{\lambda}$ so $\lambda = \frac{hc}{E} = \frac{(6.626 \;x\; 10^{-34} \;J \cdot s)(2.998 \;x\; 10^{8} \;m/s)}{1.776 \;x\; 10^{-21} \;j}$ = **$1.118 \;x\; 10^{-4}$ m or 112 µm**

This is in the far IR

So we would not expect any transitions within the H-atom to fall in the microwave region.

Problem 2.3: This problem makes use of the four- level system and associated emission lines from Figure 2.5. Assume there is an additional energy level E_5 that has an associated emission to E_4 with a wavelength of 710 nm. Sketch the energy level diagram for this five- level system, clearly labeling the energies of all $E_{excited}$ to E_1 transitions.

From Fig. 2.5 we know the wavelengths of the first three transitions, so we can get the energies:

$E_2 \rightarrow E_1$ $E = \frac{hc}{\lambda} = \frac{(6.626\ x\ 10^{-34}\ J \cdot s)(2.998\ x\ 10^{8}\frac{m}{s})}{650\ x\ 10^{-9}\ m}$ = 3.056×10^{-19} J = 3.1×10^{-19} J

$E_3 \rightarrow E_1$ $E = \frac{hc}{\lambda} = \frac{(6.626\ x\ 10^{-34}\ J \cdot s)(2.998\ x\ 10^{8}\frac{m}{s})}{530\ x\ 10^{-9}\ m}$ = 3.748×10^{-19} J = 3.8×10^{-19} J

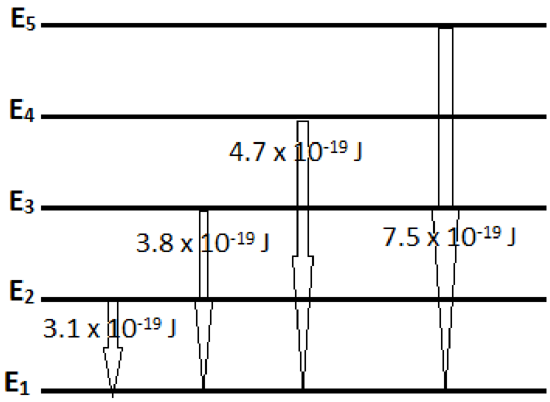
$E_4 \rightarrow E_1$ $E = \frac{hc}{\lambda} = \frac{(6.626\ x\ 10^{-34}\ J \cdot s)(2.998\ x\ 10^{8}\frac{m}{s})}{420\ x\ 10^{-9}\ m}$ = 4.729×10^{-19} J = 4.7×10^{-19} J

We know that the wavelength of the photon related to the transition between E_5 and E_4 is 710 nm, which has an energy of

$E_5 \rightarrow E_4$ $E = \frac{hc}{\lambda} = \frac{(6.626\ x\ 10^{-34}\ J \cdot s)(2.998\ x\ 10^{8}\frac{m}{s})}{710\ x\ 10^{-9}\ m}$ = 2.798×10^{-19} J

So the energy of the transition from E_5 to E_1 is the sum of the energies of E_5 to E_4 and E_4 and E_1

$E_5 \rightarrow E_1 = 4.729 \times 10^{-19}$ J + 2.798×10^{-19} J = 7.527×10^{-19} = 7.5×10^{-19} J



Problem 2.4:

(a) Calculate the reduced mass for NO and HCl.
(b) Would the reduced mass of H- ^{35}Cl be different than H- ^{37}Cl? If so, might this lead to a difference in infrared absorption? Support your response with a calculation.
(c) For Example 2.3, would you expect to measure infrared absorption for O_2?

(a) $\mu(\mathrm{NO}) = \frac{m_N \cdot m_O}{m_N + m_O} = \frac{\left(14.01\frac{g}{mol}\right) \cdot \left(16.00\frac{g}{mol}\right)}{\left(14.01\frac{g}{mol}\right) + \left(16.00\frac{g}{mol}\right)} = 7.46\underline{9}5\ \mathrm{g/mol}$

$x\ \frac{1\ kg}{1000\ g}\ x\ \frac{1\ mol}{6.022\ x\ 10^{23}\ atom} = \mathbf{1.240\ x\ 10^{-26}\ kg}$

$\mu(\mathrm{HCl}) = \frac{m_H \cdot m_{Cl}}{m_H + m_{Cl}} = \frac{\left(1.008\frac{g}{mol}\right) \cdot \left(35.45\frac{g}{mol}\right)}{\left(1.008\frac{g}{mol}\right) + \left(35.45\frac{g}{mol}\right)} = 0.980\underline{1}3\ \mathrm{g/mol}$

$x\ \frac{1\ kg}{1000\ g}\ x\ \frac{1\ mol}{6.022\ x\ 10^{23}\ atom} = \mathbf{1.628\ x\ 10^{-27}\ kg}$

(b) Yes. The reduced masses for the two isotopic forms of the HCl molecule will be different, and from equations 2.10 and 2.12, we see that a difference in μ will yield a different $\nu_{\mathrm{oscillator}}$, which is the frequency of the IR absorption.

$\mu(\mathrm{H}^{35}\mathrm{Cl}) = \frac{m_H \cdot m_{Cl}}{m_H + m_{Cl}} = \frac{\left(1.008\frac{g}{mol}\right) \cdot \left(34.969\frac{g}{mol}\right)}{\left(1.008\frac{g}{mol}\right) + \left(34.969\frac{g}{mol}\right)} = 0.979\underline{7}6\ \mathrm{g/mol}$

$x\ \frac{1\ kg}{1000\ g}\ x\ \frac{1\ mol}{6.022\ x\ 10^{23}\ atom} = \mathbf{1.627\ x\ 10^{-27}\ kg}$

$\mu(\mathrm{H}^{37}\mathrm{Cl}) = \frac{m_H \cdot m_{Cl}}{m_H + m_{Cl}} = \frac{\left(1.008\frac{g}{mol}\right) \cdot \left(36.966\frac{g}{mol}\right)}{\left(1.008\frac{g}{mol}\right) + \left(36.966\frac{g}{mol}\right)} = 1.05\underline{1}3\ \mathrm{g/mol}$

$x\ \frac{1\ kg}{1000\ g}\ x\ \frac{1\ mol}{6.022\ x\ 10^{23}\ atom} = \mathbf{1.746\ x\ 10^{-27}\ kg}$

Isotopic differences will have negligible effect on force constant, since the nuclear charge for each atom involved remains the same, as does the total electron density.

$$\frac{2\pi\nu_{H^{35}Cl}}{2\pi\nu_{H^{37}Cl}} = \sqrt{\frac{\frac{k}{\mu_{H^{35}Cl}}}{\frac{k}{\mu_{H^{37}Cl}}}} = \sqrt{\frac{\mu_{H^{37}Cl}}{\mu_{H^{35}Cl}}} = \sqrt{\frac{1.746\ x\ 10^{-27}}{1.627\ x\ 10^{-27}}} \qquad \frac{\nu_{H^{35}Cl}}{\nu_{H^{37}Cl}} = 1.036$$

So the frequency of the H-^{35}Cl absorption would be about 4% higher than that of H-^{37}Cl.

(c) We can calculate a theoretical absorption wavenumber (assuming the n=0 → n=1 transition) as
c = λν, where ν = 4.73 x 10^{13} s^{-1} from Example 2.3,

so $\lambda = \frac{c}{\nu} = \frac{2.998 \ x \ 10^{8} \ m/s}{4.73 \ x \ 10^{13} \ /s}$ = 6.34 x 10^{-6} m or 6.34 µm

However, we also know (see text following Example 2.4) that in order to observe a peak in an IR spectrum, the associated vibration must exhibit a change in dipole moment, which is not the case for O_2, so we would not expect to observe a peak for the O_2 stretching vibration.

Problem 2.5: The spring constant between atoms in HCl is around 516 N/ m. Calculate the angular frequency and vibrational frequency of HCl molecule. Determine the energy difference between the n = 0 and n = 1 states for this molecule in joules. Is this an allowed transition? What photon wavelength, in units of microns and wave numbers, would be associated with absorption from n = 0 to n = 1? Label the region of the electromagnetic spectrum.

We have the reduced mass for HCl as 1.628 x 10^{-27} kg from Problem 2.4.

$$\varpi_{osc} = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{516 \ N/m}{1.628 \ x \ 10^{-27} \ kg}} = \sqrt{\frac{516 \ (kg \cdot \frac{m}{s^{2}})/m}{1.628 \ x \ 10^{-27} \ kg}} = 5.6\underline{2}99 \ x \ 10^{14} \ rad\ /\ s$$

$$\nu_{osc} = \frac{\varpi_{osc}}{2\pi \ rad} = \frac{(5.6299 \ x \ 10^{14} \ rad/s)}{2\pi \ rad} = 8.9\underline{6}0 \ x \ 10^{13} \ s^{-1} = \mathbf{8.96 \ x \ 10^{13} \ s^{-1}}$$

For n=0 → n=1,
$\Delta E = \hbar\omega_{osc} = h\nu_{osc}$ = (6.626 x 10^{-34} J·s)(8.960 x 10^{13} s^{-1}) = 5.937 x 10^{-20} J = **5.94 x 10^{-20} J**

This is an **allowed** transition: it meets both selection rules of (1) Δn = $\underline{+}$ 1 and (2) the vibration entails a change in dipole moment.

$\lambda = \frac{hc}{E} = \frac{(6.626 \ x \ 10^{-34} \ J \cdot s) \ \cdot \ (2.998 \ x \ 10^{8} \ m/s)}{5.937 \ x \ 10^{-20} \ J}$ = 3.346 x 10^{-6} m = **3.35 µm** (around 3000 cm^{-1})

This falls in the **mid-IR** region of the EMS.

Problem 2.6: The absorption from n = 0 to n = 1 occurs at 2170 cm^{-1} in ^{12}C– ^{16}O.
(a) Calculate the spring constant between atoms in this molecule.
(b) State why this is an allowed transition.

(a) Convert $\bar{\upsilon}$ to λ: (2170 $cm^{-1})^{-1}$ = 4.6083 x 10^{-4} cm = 4.6$\underline{0}$83 x 10^{-6} m

Convert λ to ν: c = λν $2.998\text{x}10^{8}$ m/s = ($4.6\underline{0}83 \text{ x } 10^{-6}$ m)(ν) ν = $6.5\underline{0}566 \text{ x } 10^{13}$ s^{-1}
Convert ν to ω: ω = 2πν = 2π($6.5\underline{0}566 \text{ x } 10^{13}$ s^{-1}) = $4.0\underline{8}76 \text{ x } 10^{14}$ rad/s

Convert ω to k: $\mu = \dfrac{mm}{m+m} = \dfrac{(12 x 16)}{12+16}$ = 6.857 g/mol $x \dfrac{1 \ mol}{6.022 \ x \ 10^{23} \ atoms} \ x \ \dfrac{1 \ kg}{1000 \ g}$
= $1.1387 \text{ x } 10^{-26}$ kg

$\omega = \sqrt{\dfrac{k}{\mu}}$ **k = 1902.6 = 1.90 x 10^{3} N/m**

(b) Since this is a heteroatomic molecule, the stretching vibration will exhibit a change in dipole moment.

Problem 2.7: The frequency spacing between rotational levels is 511 MHz in HBr. Calculate the difference in energy of the J = 0 and J = 1 states. Calculate the bond length for HBr.

E= hν = ($6.626 \text{ x } 10^{-34}$ J·s) ($511 \text{ x } 10^{6}$ s^{-1}) = $3.386 \text{ x } 10^{-25}$ J = **3.39 x 10^{-25} J**

$$\Delta E = J(J+1)\frac{\hbar^2}{2\mu R_0^2}$$

$$\mu = \frac{(1.008)(79.90)}{(1.008)+(79.90)}\frac{g}{mol} x \frac{1 \ kg}{1000 \ g} \ x \ \frac{1 \ mol}{6.022 \ x \ 10^{23} molecules} = 1.653 \text{ x } 10^{-27} \text{ kg}$$

$$R_0^2 = J(J+1)\frac{\hbar^2}{2\mu\Delta E} = 1(1+1)\frac{(1.05 \ x \ 10^{-34} \ J\cdot s)^2}{(2)(1.653 \ x \ 10^{-27} \ kg)(3.386 \ x \ 10^{-25} \ J)} = 9.849 \text{ x } 10^{-18} \text{ m}^2$$

$R =$ $3.138 \text{ x } 10^{-9}$ m = **31.4 Å = bond length**

Problem 2.8: Rotational absorption is observed at 0.13 cm for the CO molecule. The transition is associated with the J=1 to J=2 energy levels. Use this information to estimate the rotational inertia for CO.

$$\Delta E = \frac{hc}{\lambda} = \frac{(6.626 \ x \ 10^{-34} \ J\cdot s)(2.998 \ x \ 10^{8}\frac{m}{s})}{0.13 \ x \ 10^{-2} \ m} = 1.\underline{5}28 \text{ x } 10^{-22} \text{ J}$$

$$\Delta E = J_2(J_2+1)\frac{\hbar^2}{2I} - J_1(J_1+1)\frac{\hbar^2}{2I}$$

$$\Delta E = 2(2+1)\frac{\hbar^2}{2I} - 1(1+1)\frac{\hbar^2}{2I}$$

$$\Delta E = 6\ \frac{\hbar^2}{2I} - \ 2\ \frac{\hbar^2}{2I} = 4\ \frac{\hbar^2}{2I}$$

$$I = 4\ \frac{\hbar^2}{2\Delta E} = \quad 4\ \frac{(1.0545\ \ x\ \ 10^{-34}\ \ J\cdot s)^2}{2\ (1.528\ \ x\ \ 10^{-22}\ \ J)} = \ 1.455\ \ x\ \ 10^{-46}\ \ J\cdot s^2 = \ 1.5\ \ x\ \ 10^{-46}\ \ J\cdot s^2$$

Problem 2.9: Suppose two different states (with no degeneracy so that $g_1 = g_2 = 1$) have energies $E_2 = 2 \times 10^{-22}$ J and $E_1 = 0.5 \times 10^{-22}$ J. At what temperature will N_2 have a population will $N_2/N_1 = 100$? Suppose now that the degeneracies are $g_1 = 3$, $g_2 = 2$. Is it possible to find a temperature where the population in N_2 is larger than N_1?

$\Delta E = 2 \text{ x } 10^{-22} - 0.5 \text{ x } 10^{-22}$ J $= 1.5 \text{ x } 10^{-22}$ J

$$\frac{N_2}{N_1} = \frac{g_2}{g_1}\ e^{\left(\frac{-\Delta E}{k_B T}\right)} = \frac{1}{1}\ e^{\left(\frac{-1.5\ \ x\ \ 10^{-22}}{(1.38\ \ x\ \ 10^{-23} J/K)(T)}\right)} = 100$$

$$\left(\frac{-1.5\ \ x\ \ 10^{-22}}{(1.38\ \ x\ \ 10^{-23} J/K)(T)}\right) = 4.605$$

T = –2.36 K That is, it is not possible for the population ratio N_2/N_1 to equal 100.

When $g_1 = 3$ and $g_2 = 2$, can $N_2 > N_1$? If we solve the fundamental equation for temperature, we can get a handle on this question:

$$T = \frac{\frac{-\Delta E}{k_B}}{\ln\left(\frac{N_2}{N_1}\ \cdot\ \frac{g_1}{g_2}\right)}$$

When $g_1 = 3$ and $g_2 = 2$, the function $\ln\left(\frac{N_2}{N_1}\ \cdot\ \frac{g_1}{g_2}\right)$ will be positive whenever $N_2 > N_1$, which would yield a negative Kelvin temperature; Thus, it is not possible for N_2 to exceed N_1 in this case.

Problem 2.10: Suppose an electron is trapped in one dimension to a length of 2 nm, the length of some polymer.

(a) What is the wavelength absorbed by such a system from the ground state to the first excited state? *Hint*: This can be modeled as a particle in a one- dimensional box.

(b) How does the length of the polymer (the length of the box) affect the absorption wavelength from the ground state to the first excited state? In order to answer this question, use a spreadsheet to calculate the wavelengths associated with this transition for one- dimensional boxes that are from 1 to 200 nm in size at intervals of 10 nm. Make a plot of wavelength of absorption versus polymer length.

(a) In Footnote 11 (page 42) we are given the pertinent equation for the energy of a particle in a box:

$$E_n = \frac{h^2 n^2}{8 m a^2}$$

where n is the principal quantum number, m is the mass, and a is the length of the one-dimensional box. After we calculate the energy, we can use Eq. 2.4 to convert to wavelength.

$$\Delta E = \frac{h^2 n_2^2}{8 m a^2} - \frac{h^2 n_1^2}{8 m a^2} = \frac{h^2}{8 m a^2}(n_2^2 - n_1^2)$$

where, in this case, $n_1 = 1$ (ground state) and $n_2 = 2$ (first excited state)

$m = 9.1094 \ x \ 10^{-31} \ kg$ (the mass of an electron)

$a = 2 \ nm \ x \ \frac{1 \ m}{10^9 \ nm}$ = 2 x 10^{-9} m

$$\Delta E = \frac{(6.626 \ x \ 10^{-34} \ J \cdot s)^2}{8 \cdot (9.1094 \ x \ 10^{-31} kg)(2 \ x \ 10^{-9} m)^2}(2^2 - 1^2) = \underline{4}.52 \ x \ 10^{-20} \ J = E_{photon}$$

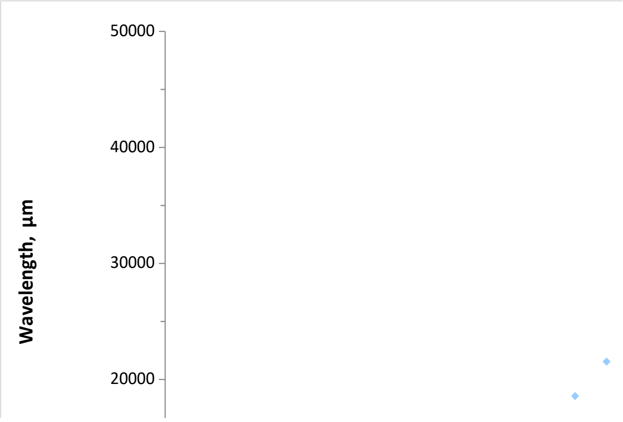
$$\lambda = \frac{hc}{E} = \frac{(6.626 \ x \ 10^{-34} J \cdot s)(2.998 \ x \ 10^8 \frac{m}{s})}{4.52 \ x \ 10^{-20} \ J} = 4.396 \ x \ 10^{-6} \ m = \mathbf{\underline{4}.4 \ \mu m}$$

(b)

h =

c =

a (nm)



As expected, the wavelength of the absorbed light increases as the square of the "box" length.

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Problem 2.11: Carbon- 13 (^{13}C) has a gyromagnetic ratio of 6.73×10^{7} T^{-1}, s^{-1}. Repeat Example 2.8 for a carbon-13 nucleus.

Using B = 3 T, assuming that is an exact number.

$\Delta E = \hbar\gamma B = (1.0546 \ x \ 10^{-34} J \cdot s)(6.73 \ x \ 10^{7} \ T^{-1} s^{-1})(3 \ T)$ = $2.129 \text{ x } 10^{-26}$ J

E = hν ν = $3.213 \text{ x } 10^{7} s^{-1}$ = 32.13 MHz

c = λν λ = 9.31 m

Problem 2.12: Carbon- 13 (^{13}C) has a gyromagnetic ratio of 6.73×10^{7} T^{-1}, s^{-1}. Repeat Example 2.9 for a carbon-13 nucleus.

$\Delta E = \hbar\gamma B = (1.0546 \ x \ 10^{-34} J \cdot s)(6.73 \ x \ 10^{7} \ T^{-1} s^{-1})(1.258 \ T)$ = $8.9286 \text{ x } 10^{-27}$ J

E = hν ν = $1.3475 \text{ x } 10^{7} s^{-1}$

c = λν λ = 22.25 m

$\Delta E = \hbar\gamma B = (1.0546 \ x \ 10^{-34} J \cdot s)(6.73 \ x \ 10^{7} \ T^{-1} s^{-1})(1.257 \ T)$ = $8.9215 \text{ x } 10^{-27}$ J

E = hν ν = $1.346 \text{ x } 10^{7} s^{-1}$

c = λν λ = 22.27 m

Problem 2.13: You are considering purchasing a new NMR instrument so that you can do ^{1}H NMR. Suppose one instrument would provide a magnetic field of 10 T and another would provide a field of 3 T. For a given molecule, would these two instruments have two different absorption wavelengths between spin states? If so, calculate the two different wavelengths that would cause absorption, ignoring the internal magnetic field of the molecule.

Yes, the energy (an thus, the wavelength) is dependent on the magnetic field strength, B. Following Example 2.8, and using B = 10 T, assuming that is an exact number.

$\Delta E = \hbar\gamma B = (1.0546 \ x \ 10^{-34} J \cdot s)(2.675 \ x \ 10^{8} \ T^{-1} s^{-1})(10 \ T)$ = $2.821 \text{ x } 10^{-25}$ J

$$\lambda = \frac{hc}{E} = \frac{(6.626 \ x \ 10^{-34} J \cdot s)(2.998 \ x \ 10^{8} \frac{m}{s})}{2.821 \ x \ 10^{-25} \ J} = 0.704 \text{ m}$$

We can compare this to the wavelength of 2.36 m obtained in Example 2.8 for B = 3 T.

EXERCISE 2.1: The spring constant associated with NO is 1530 N/ m. Calculate the frequency of oscillation for this molecule.

$$\mu = \frac{mm}{m+m} = \frac{(14.01 \ x \ 16.00)}{14.01 + 16.00} = 7.4695 \text{ g/mol} \ x \ \frac{1 \ mol}{6.022 \ x \ 10^{23} \ atoms} \ x \ \frac{1 \ kg}{1000 \ g}$$

$= 1.24\underline{0}4 \text{ x } 10^{-26}$ kg

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{1530 \ kg \cdot \frac{m}{s} / m}{1.2404 \ x \ 10^{-26} \ kg}} = 3.5\underline{1}21 \text{ x } 10^{14} \text{ rad/s}$$

$v = \frac{\omega}{2\pi}$ = 5.5897 x 10^{13} s^{-1} = **5.59 x 10^{13} s^{-1}**

EXERCISE 2.2: The spring constant of the diatomic molecule NO is 1530 N/ m.
(a) Calculate the energy level difference from n = 0 to n = 1
(b) Calculate the energy level difference from n = 1 to n = 2.

We have ω = $3.5\underline{1}21$ x 10^{14} rad/s for NO from Exercise 2.1.

(a) $\Delta E = E_2 - E_1 = (1 + ½)\hbar\omega - (0 + ½)\hbar\omega = (1)\hbar\omega = (1.0546 \text{ x } 10^{-34} \text{ J·s})(3.5121 \text{ x } 10^{14} \text{ s}^{-1})$
= 3.703 x 10^{-20} J = **3.70 x 10^{-20} J**

(b) $\Delta E = E_2 - E_1 = (2 + ½)\hbar\omega - (1 + ½)\hbar\omega = (1)\hbar\omega = (1.0546 \text{ x } 10^{-34} \text{ J·s})(3.5121 \text{ x } 10^{14} \text{ s}^{-1})$
= 3.703 x 10^{-20} J = **3.70 x 10^{-20} J**

As indicated by Figure 2.8, the energy difference between adjacent vibrational energy levels is constant.

EXERCISE 2.3: The spring constant associated with CO is 1860 N/ m. Calculate the frequency of oscillation for this molecule.

$$\mu = \frac{mm}{m+m} = \frac{(12.01 \ x \ 16.00)}{12.01+16.00} = 6.86\underline{0}4 \text{ g/mol } x \ \frac{1 \ mol}{6.022 \ x \ 10^{23} \ atoms} \ x \ \frac{1 \ kg}{1000 \ g}$$

= $1.13\underline{9}2$ x 10^{-26} kg

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{1860 \ kg \cdot \frac{m}{s}/m}{1.1392 \ x \ 10^{-26} \ kg}} = 4.0\underline{4}066 \text{ x } 10^{14} \text{ rad/s}$$

$v = \frac{\omega}{2\pi}$ = $6.4\underline{3}1$ x 10^{13} s^{-1} = **6.43 x 10^{13} s^{-1}**

EXERCISE 2.4: The molecular vibration of HF is well described with a spring constant of 970 N/m. What is the wavelength of photon absorbed from the n = 1 to n = 2 states?

$$\mu = \frac{mm}{m+m} = \frac{(1.008 \, x \, 19.00)}{1.008+19.00} = 0.9572 \text{ g/mol } x \ \frac{1 \ mol}{6.022 \ x \ 10^{23} \ atoms} \ x \ \frac{1 \ kg}{1000 \ g}$$

= $1.58\underline{9}8$ x 10^{-27} kg

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{970 \ kg \cdot \frac{m}{s}/m}{1.5898 \ x \ 10^{-27} \ kg}} = 7.8\underline{1}18 \text{ x } 10^{14} \text{ rad/s}$$

$v = \frac{\omega}{2\pi}$ = 1.2$\underline{4}$3 x 10^{14} s^{-1}

$\Delta E = E_2 - E_1 = (2 + ½)ħω – (1 + ½)\ ħω = (1)\ ħω = (1.0546 \times 10^{-34}\ J\cdot s)(7.8118 \times 10^{14}\ s^{-1})$

= 8.2383 x 10^{-20} J

$E = \frac{hc}{\lambda}$ λ = 2.41 μm

EXERCISE 2.5: Using spreadsheet software, calculate the energies for vibrational states from n=0 to n=10 for HI. HI has a spring constant of 320 N/ m. Using your spreadsheet, calculate the energy level differences between adjacent levels up to n=10.

For n=0:

Using the vibrational energy level equation

$\mu = \frac{mm}{m+m} = \frac{(1.008\,x\,126.90)}{1.008+126.90}$ = 1.00$\underline{0}$05 g/mol $x\ \frac{1\ \ mol}{6.022\ \ x\ \ 10^{23}\ \ atoms}\ x\ \frac{1\ \ kg}{1000\ \ g}$

= 1.66$\underline{0}$7 x 10^{-27} kg

$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{320\ \ kg\cdot\frac{m}{s}/m}{1.6607\ \ x\ \ 10^{-27}\ \ kg}}$ = 4.38$\underline{9}$7 x 10^{14} rad/s

$E = \left(n+\frac{1}{2}\right)ħ\omega = (0+\frac{1}{2})(1.0546\ \ x\ \ 10^{-34}\ \ J\cdot s)(4.3897\ \ x\ \ 10^{14} rad/s)$ = 2.31$\underline{4}$6 x 10^{-20} J

Further calculations done in the spreadsheet:

ħ = 1.0546E-34		ω = 4.3897E+14	
n	E (J)	ΔE (J)	
0	2.315E-20		
1	6.944E-20	4.629E-20	
2	1.157E-19	4.629E-20	
3	1.620E-19	4.629E-20	
4	2.083E-19	4.629E-20	
5	2.546E-19	4.629E-20	
6	3.009E-19	4.629E-20	
7	3.472E-19	4.629E-20	
8	3.935E-19	4.629E-20	
9	4.398E-19	4.629E-20	
10	4.861E-19	4.629E-20	
11	5.324E-19	4.629E-20	
12	5.787E-19	4.629E-20	
13	6.249E-19	4.629E-20	
14	6.712E-19	4.629E-20	
15	7.175E-19	4.629E-20	
16	7.638E-19	4.629E-20	
17	8.101E-19	4.629E-20	
18	8.564E-19	4.629E-20	
19	9.027E-19	4.629E-20	
20	9.490E-19	4.629E-20	
21	9.953E-19	4.629E-20	

EXERCISE 2.6: It can be quite useful to move beyond the simple harmonic oscillator model of diatomic molecules. Using the Morse potential, a more accurate model for the molecular potential that takes into account the asymmetric molecular potential, the energy levels are:

$$E=\left(n+\frac{1}{2}\right)\hbar\omega-\frac{(h\upsilon)^2}{4D_e}\left(n+\frac{1}{2}\right)^2$$

where D_e is the bond energy (the energy from the minimum of the potential the energy at which the bond is broken). Note that the first term in the equation is what we found using the simple harmonic oscillator potential. The second term is often referred to as the anharmonic correction.

The dissociation energy for CO is 11.2 eV (1.79×10^{-18} J) the force constant is 1860 N/ m. Calculate the energy difference between the ground state and the first excited state two ways, with the energy equation for the simply harmonic oscillator and with the anharmonic correction. How large is the correction associated with the anharmonic potential?

The reduced mass of a CO molecule is $1.13\underline{9}2 \times 10^{-26}$ kg.

$$\omega=\sqrt{\frac{k}{\mu}}=\sqrt{\frac{1860\ \frac{kg\cdot m}{m\cdot s^2}}{1.1392\ x\ 10^{-26}\ kg}} = 4.0\underline{4}07 \times 10^{14}\ \text{rad/s}$$

$v=\frac{\omega}{2\pi}$ = 6.43097 x 10^{13} s^{-1}

Using the simple harmonic oscillator model:
$\Delta E = E_2 - E_1 = (1 + \frac{1}{2})\hbar\omega - (0 + \frac{1}{2})\hbar\omega = (1)\hbar\omega = (1.0546 \text{ x } 10^{-34}\ J\cdot s)(4.0\underline{4}07 \text{ x } 10^{14}\ s^{-1})$
$\Delta E = 4.261 \text{ x } 10^{-20}$ J = $4.26 \text{ x } 10^{-20}$ J

Using the Morse model:
$E_{(n=0)}$ = $\left(n+\frac{1}{2}\right)\hbar\omega$ - $\frac{(hv)^2}{4D_e}\cdot\left(n+\frac{1}{2}\right)^2$
$E_{(n=0)}$
$$= \left(0+\frac{1}{2}\right)(1.0546\ \ x\ \ 10^{-34}J\cdot s)(4.0407\ \ x\ \ 10^{14}s^{-1}) - \frac{((6.626\ \ x\ \ 10^{-34}J\cdot s)(6.431\ \ x\ \ 10^{13}s^{-1})^2}{4(1.79\ \ x\ \ 10^{-18}J)}\cdot(0+\frac{1}{2})^2$$
$E_{(n=0)}$ = $2.13066 \text{ x } 10^{-20}$ J – $6.339965 \text{ x } 10^{-23}$ J = $2.1243 \text{ x } 10^{-20}$ J

$E_{(n=1)}$ = $\left(1+\frac{1}{2}\right)\hbar\omega$ - $\frac{(hv)^2}{4D_e}\cdot\left(1+\frac{1}{2}\right)^2$
$E_{(n=0)}$
$$= \left(1+\frac{1}{2}\right)(1.0546\ \ x\ \ 10^{-34}J\cdot s)(4.0407\ \ x\ \ 10^{14}s^{-1}) - \frac{((6.626\ \ x\ \ 10^{-34}J\cdot s)(6.431\ \ x\ \ 10^{13}s^{-1})^2}{4(1.79\ \ x\ \ 10^{-18}J)}\cdot(1+\frac{1}{2})^2$$
$E_{(n=0)}$ = $6.3915 \text{ x } 10^{-20}$ J – $5.70597 \text{ x } 10^{-22}$ J = $6.3344 \text{ x } 10^{-20}$ J

$\Delta E = (6.3344 - 2.1243) \text{ x } 10^{-20}$ J = $4.210 \text{ x } 10^{-20}$ J

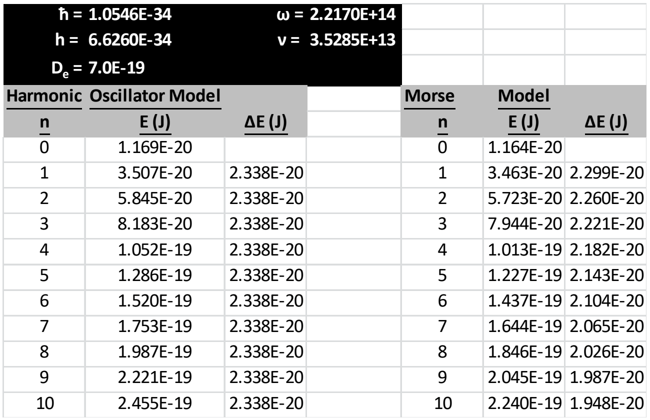
Assuming the Morse model is the more accurate (i.e., the true value),
$\%\ \ difference = \frac{4.261 - 4.210}{4.210}\ \ x\ \ 100\,\%$ = 1.45% difference

EXERCISE 2.7: For two cases, using the energy levels from the harmonic oscillator and then with the full Morse potential energy state, use spreadsheet software to produce a plot of energy level difference for vibration as a function of quantum number n. Describe the relationship and discuss the role of the anharmonic correction. Use values for HCl for your calculation (k = 80 N/ m, disassociation energy = 7.0 × 10^{-19} J).

The reduced mass of the HCl molecule is $1.62\underline{7}6 \text{ x } 10^{-27}$ kg.

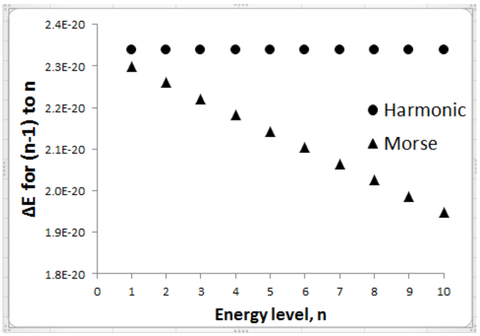
$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{80\ \ \frac{kg\cdot m}{m\cdot s^2}}{1.6276\ \ x\ \ 10^{-27}\ \ kg}} = 2.\underline{2}17 \text{ x } 10^{14} \text{ rad/s}$$
$v=\frac{\omega}{2\pi}$ = $3.\underline{5}285 \text{ x } 10^{13}$ s^{-1}

We will use a spreadsheet and calculations demonstrated in Ex. 2.6 to create the desired plots.



$\hbar$ = 1.0546E-34 ω = 2.2170E+14
h = 6.6260E-34 ν = 3.5285E+13
D_e = 7.0E-19

Harmonic	Oscillator Model			Morse	Model	
n	E (J)	ΔE (J)		n	E (J)	ΔE (J)
0	1.169E-20			0	1.164E-20	
1	3.507E-20	2.338E-20		1	3.463E-20	2.299E-20
2	5.845E-20	2.338E-20		2	5.723E-20	2.260E-20
3	8.183E-20	2.338E-20		3	7.944E-20	2.221E-20
4	1.052E-19	2.338E-20		4	1.013E-19	2.182E-20
5	1.286E-19	2.338E-20		5	1.227E-19	2.143E-20
6	1.520E-19	2.338E-20		6	1.437E-19	2.104E-20
7	1.753E-19	2.338E-20		7	1.644E-19	2.065E-20
8	1.987E-19	2.338E-20		8	1.846E-19	2.026E-20
9	2.221E-19	2.338E-20		9	2.045E-19	1.987E-20
10	2.455E-19	2.338E-20		10	2.240E-19	1.948E-20



The simple harmonic oscillator predicts that the energy difference between successive energy levels remains constant; with the Morse model, we can see that difference between energy levels decreases slightly as n increases – that is, the energy levels get closer to each other as n increases. We would expect this to be the case, because as n increases, at some point we expect the bond energy to be exceeded, causing the bond to break.

EXERCISE 2.8: The disassociation energy for NO is 7.0 eV (1.12×10^{-18} J) and the effective spring constant is 1530 N/ m. Calculate the energy level difference between the n = 5 and n = 6 states and the associated absorption wavelength using the harmonic oscillator model and the Morse potential model (see Exercise 2.7).

The reduced mass of a NO molecule is 1.24$\underline{0}$4 x 10^{-26} kg.

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{1530 \ \frac{kg \cdot m}{m \cdot s^2}}{1.2404 \ x \ 10^{-26} \ kg}} = 3.5\underline{1}2 \text{ x } 10^{14} \text{ rad/s}$$

$$v = \frac{\omega}{2\pi} = 5.5\underline{8}97 \text{ x } 10^{13} \text{ s}^{-1}$$

Using the simple harmonic oscillator model:

$\Delta E = E_2 - E_1 = (6 + ½)\hbar\omega - (5 + ½)\hbar\omega = (1)\hbar\omega = (1.0546 \text{ x } 10^{-34} \text{ J·s})(3.512 \text{ x } 10^{14} \text{ s}^{-1})$

$\Delta E = 3.70376 \text{ x } 10^{-20} \text{ J} = 3.70 \text{ x } 10^{-20} \text{ J}$

$$E = \frac{hc}{\lambda} \qquad \lambda = 5.36 \ \mu\text{m}$$

Using the Morse model:

$$E_{(n=5)} = \left(5+\frac{1}{2}\right)\hbar\omega - \frac{(h\nu)^2}{4D_e}\cdot\left(5+\frac{1}{2}\right)^2$$

$E_{(n=5)}$

$$= \left(5+\frac{1}{2}\right)(1.0546 \ x \ 10^{-34} J \cdot s)(3.512 \ x \ 10^{14} s^{-1}) - \frac{\left((6.626 \ x \ 10^{-34} J \cdot s)(5.5897 \ x \ 10^{13} s^{-1})\right)^2}{4(1.12 \ x \ 10^{-18} J)} \cdot \left(5+\frac{1}{2}\right)^2$$

$E_{(n=5)}$ = 2.0371 x 10^{-19} J – 9.26247x 10^{-21} J = 1.9444x 10^{-19} J

$E_{(n=6)}$ = $\left(6+\frac{1}{2}\right)\hbar\omega$ - $\frac{(h\nu)^2}{4D_e}\cdot\left(6+\frac{1}{2}\right)^2$

$E_{(n=6)}$

= $\left(6+\frac{1}{2}\right)(1.0546\ x\ 10^{-34}\,J\cdot s)(3.512\ x\ 10^{14}\,s^{-1})$- $\frac{((6.626\ x\ 10^{-34}\,J\cdot s)(5.5897\ x\ 10^{13}\,s^{-1})^2}{4(1.12\ x\ 10^{-18}\,J)}\cdot(6+\frac{1}{2})^2$

$E_{(n=6)}$ = 2.4074 x 10^{-19} J – 1.2936 x 10^{-20} J = 2.2780 x 10^{-19} J

ΔE = (2.2780 – 1.9444) x 10^{-19} J = 3.336 x 10^{-20} J

$E=\frac{hc}{\lambda}$ λ = 5.96 μm

EXERCISE 2.9: A gas sample is thought to be either LiBr or LiI. For both molecules calculate the difference in energy due to rotation alone between J = 0 and J = 1. Then compare your answer to the energy due to rotation alone between J = 1 and J = 2 states. Are these energies above or below the thermal energy of 0.04 eV?

The reduced mass of LiBr is 1.0603 x 10^{-26} kg.
Lithium's ionic radius is 90 pm and Bromide is 182 pm or the equilibrium separation is
$R_o = 90+182 = 272\,pm$

$$E= J(J+1)\frac{\hbar^2}{2\mu R_0^2}$$

$\Delta E_{1,0}=1(1+1)\frac{\left(1.0546\ x\ 10^{-34}\frac{kg\cdot m^2}{s}\right)^2}{2(1.0603\ X\ 10^{-26}kg)(272\ x\ 10^{-12}m)^2}-0$ = 1.4178 x 10^{-23} J

eV = $1.4178\ x\ 10^{-23}J\ x\ \frac{1\ eV}{1.6022\ x\ 10^{-19\ J}}$ = 8.85 x 10^{-5} eV

$\Delta E_{2,1}=2(2+1)\frac{\left(1.0546\ x\ 10^{-34}\frac{kg\cdot m^2}{s}\right)^2}{2(1.0603\ X\ 10^{-26}kg)(272\ x\ 10^{-12}m)^2}-1(1+1)\frac{\left(1.0546\ x\ 10^{-34}\frac{kg\cdot m^2}{s}\right)^2}{2(1.0603\ X\ 10^{-26}kg)(272\ x\ 10^{-12}m)^2}$

= 5.671 x 10^{-23} J

eV = $5.671\ x\ 10^{-23}J\ x\ \frac{1\ eV}{1.6022\ x\ 10^{-19\ J}}$ = 3.54x 10^{-4} eV

Both are well below the thermal energy of 4 x 10^{-2} eV.

The reduced mass of LiI is 1.093 x 10^{-26} kg.
Lithium's ionic radius is 90 pm and Bromide is 206 pm or the equilibrium separation is

$$R_o = 90 + 206 = 296\ pm$$

$$E = \ J(J+1)\frac{\hbar^2}{2\mu R_0^2}$$

$$\Delta E_{1,0} = 1(1+1)\frac{\left(1.0546\ \ x\ \ 10^{-34}\frac{kg\cdot m^2}{s}\right)^2}{2(1.093\ \ X\ \ 10^{-26}kg)(296\ \ x\ \ 10^{-12}m)^2} - 0$$ = 1.161 x 10^{-23} J

eV = $1.161\ \ x\ \ 10^{-23}J\ \ x\ \ \frac{1\ \ eV}{1.6022\ \ x\ \ 10^{-19\ J}}$ = 7.25 x 10^{-5} eV

$$\Delta E_{2,1} = 2(2+1)\frac{\left(1.0546\ \ x\ \ 10^{-34}\frac{kg\cdot m^2}{s}\right)^2}{2(1.093\ \ X\ \ 10^{-26}kg)(296\ \ x\ \ 10^{-12}m)^2} - 1(1+1)\frac{\left(1.0546\ \ x\ \ 10^{-34}\frac{kg\cdot m^2}{s}\right)^2}{2(1.093\ \ X\ \ 10^{-26}kg)(296\ \ x\ \ 10^{-12}m)^2}$$

= 4.644 x 10^{-23} J

eV = $4.644\ \ x\ \ 10^{-23}J\ \ x\ \ \frac{1\ \ eV}{1.6022\ \ x\ \ 10^{-19\ J}}$ = 2.90 x 10^{-4} eV

Both are well below the thermal energy of 4 x 10^{-2} eV.

EXERCISE 2.10: We have now plotted energy level diagrams for several systems (hydrogen atom, vibrating diatomic molecules, and rotating diatomic molecules) in this chapter. Make such an energy level sketch of the particle in a box system described in Problem 2.10.

In Problem 2.10, we determined the energy for the transition from the ground state (n=1) to the first excited state (n=2) thus:

$m = 9.1094\ \ x\ \ 10^{-31}\ \ kg$ (the mass of an electron)

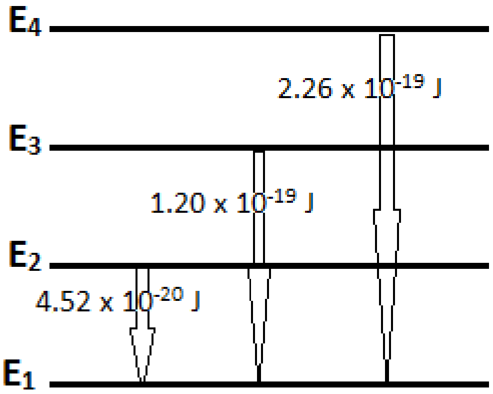
$a = 2\ \ nm\ \ x\ \ \frac{1\ \ m}{10^9\ nm}$ = 2 x 10^{-9} m

$\Delta E_{2,1} = \ \frac{(6.626\ \ x\ \ 10^{-34}\ \ J\cdot s)^2}{8\cdot(9.1094\ \ x\ \ 10^{-31}kg)(2\ \ x\ \ 10^{-9}m)^2}(2^2-1^2)$ = $\underline{4}$.52 x 10^{-20} J = E_{photon}

We can do this for the next few energy levels:

$\Delta E_{3,1} = \ \frac{(6.626\ \ x\ \ 10^{-34}\ \ J\cdot s)^2}{8\cdot(9.1094\ \ x\ \ 10^{-31}kg)(2\ \ x\ \ 10^{-9}m)^2}(3^2-1^2)$ = $\underline{1}$.20 x 10^{-19} J = E_{photon}

$\Delta E_{4,1} = \ \frac{(6.626\ \ x\ \ 10^{-34}\ \ J\cdot s)^2}{8\cdot(9.1094\ \ x\ \ 10^{-31}kg)(2\ \ x\ \ 10^{-9}m)^2}(4^2-1^2)$ = $\underline{2}$.26 x 10^{-19} J = E_{photon}



EXERCISE 2.11: At what temperature might you expect to have populated an excited state E_2 to about 10% of N_1 from a ground state E_1 when the energy level difference is 5×10^{-20} J? What wavelength photon would be associated with the absorption between these two states? Degeneracies can be assumed to be one.

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} e^{-\frac{\Delta E}{kT}}$$

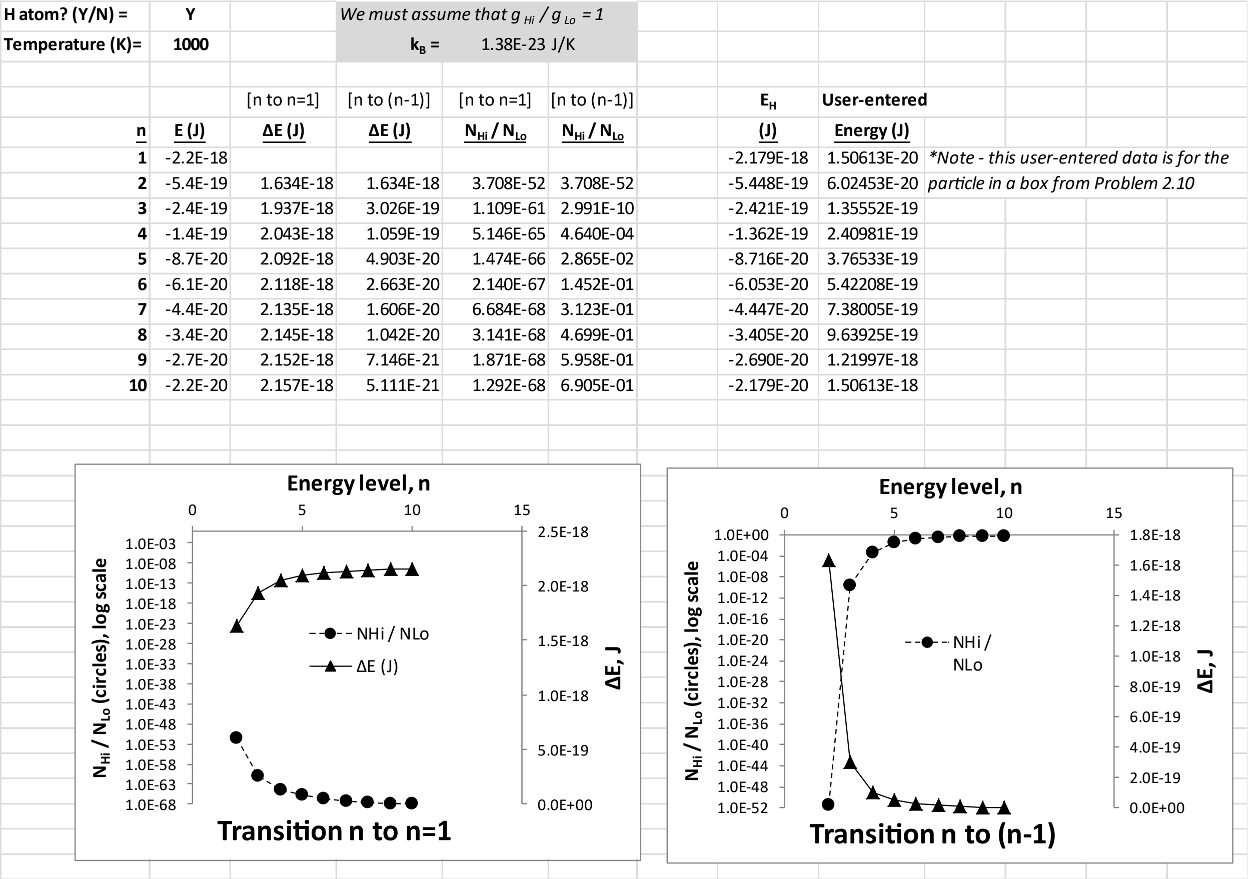
$$0.10 = (1)\ e^{-\frac{5\ x\ 10^{-20}}{(1.38\ x\ 10^{-23} J/k)T}}$$

$$-2.3026 = -\frac{5\ x\ 10^{-20} J}{\left(1.38\ x\ 10^{-23}\frac{J}{K}\right)T}$$

T = 1573 K = 1300 °C

$$E = \frac{hc}{\lambda} \qquad \lambda = 3.97\ \mu\text{m}$$

EXERCISE 2.12: Produce a spreadsheet tool that can be used to investigate the relationship between temperature, energy level difference, and populations in N_1 and N_2. Your tool should allow you to input the temperature and then plot the ratio of the populations for a range of energy level differences. What other relationships can you explore with your tool?



H atom? (Y/N) =	**Y**		*We must assume that g_{Hi} / g_{Lo} = 1*						
Temperature (K)=	**1000**			k_B = 1.38E-23 J/K					
		[n to n=1]	[n to (n-1)]	[n to n=1]	[n to (n-1)]		E_H	**User-entered**	
n	**E (J)**	**ΔE (J)**	**ΔE (J)**	**N_{Hi} / N_{Lo}**	**N_{Hi} / N_{Lo}**		**(J)**	**Energy (J)**	
1	-2.2E-18						-2.179E-18	1.50613E-20	**Note - this user-entered data is for the*
2	-5.4E-19	1.634E-18	1.634E-18	3.708E-52	3.708E-52		-5.448E-19	6.02453E-20	*particle in a box from Problem 2.10*
3	-2.4E-19	1.937E-18	3.026E-19	1.109E-61	2.991E-10		-2.421E-19	1.35552E-19	
4	-1.4E-19	2.043E-18	1.059E-19	5.146E-65	4.640E-04		-1.362E-19	2.40981E-19	
5	-8.7E-20	2.092E-18	4.903E-20	1.474E-66	2.865E-02		-8.716E-20	3.76533E-19	
6	-6.1E-20	2.118E-18	2.663E-20	2.140E-67	1.452E-01		-6.053E-20	5.42208E-19	
7	-4.4E-20	2.135E-18	1.606E-20	6.684E-68	3.123E-01		-4.447E-20	7.38005E-19	
8	-3.4E-20	2.145E-18	1.042E-20	3.141E-68	4.699E-01		-3.405E-20	9.63925E-19	
9	-2.7E-20	2.152E-18	7.146E-21	1.871E-68	5.958E-01		-2.690E-20	1.21997E-18	
10	-2.2E-20	2.157E-18	5.111E-21	1.292E-68	6.905E-01		-2.179E-20	1.50613E-18	

EXERCISE 2.13: You are doing proton NMR and would like to investigate the role of the magnetic field on the ratio of populations N_2/N_1 between two spin states in proton NMR at 300K. Ignore any particular local magnetic field contributions for the molecule being investigated. Use a spreadsheet tool to produce a plot of N_1/ N_2 as a function of magnetic field. Use your tool to determine the B field at which $N_1 = 1.02\ N_2$. The largest NMR magnets can achieve a B field of around 23 T. Comment on the viability of getting to your B field.

γ_H =	**2.675E+08**	**$(Ts)^{-1}$**
ħ =	**1.055E-34**	**J·s**
k_B =	**1.38E-23**	**J/K**
T =	**300**	**K**
B (T)	**N_2/N_1**	**N_1/N_2**
1	0.999993	1.000007
5	0.999966	1.000034
10	0.999932	1.000068
15	0.999898	1.000102
20	0.999864	1.000136
25	0.999830	1.00017
30	0.999796	1.000204
3000	0.979765	1.020653

We would need a field of B = 3,000 T in order to achieve N_1/N_2 = 1.02. With current technology, this is not possible.