Solutions to:

Atomic Structrure Homework Problem Set
Chemistry 145, Chapter 7

1. Carbon dioxide (CO2) in the atmosphere acts as a greenhouse gas by absorbin infrared radiation at a wavelength of 15 µm. What is the frequency of this radiation (Hz)? What is the energy of a single photon of this radiation (J)? What is the energy of a mole of photons at this wavelength (J mole -1)?

Constants:

$\mu m := 10^{-6} \cdot m$ $\quad$ $c := 2.99792458 \cdot 10^{8} \cdot m \cdot sec^{-1}$

$kJ := 10^{3} \cdot joule$ $\quad$ $h := 6.6260755 \cdot 10^{-34} \cdot joule \cdot sec$

$N := 6.0221367 \cdot 10^{23} \cdot mole^{-1}$

Given:

$\lambda := 15 \cdot \mu m$

What is the frequency of this radiation?

$c = \lambda \cdot \nu$ — Equation that relates the speed (c), wavelength (λ) and frequency (ν) of light.

$\nu := \frac{c}{\lambda}$ — Rearanged to solve for the frequency.

$\nu = 1.999 \cdot 10^{13} \cdot sec^{-1}$

$\nu = 1.999 \cdot 10^{13} \cdot Hz$

What is the energy of a single photon of this radiation (J)

$E := h \cdot \nu$ — Equation that relates the energy (E) and frequency (ν) of radiation using Plank's constant (h)

$E = 1.324 \cdot 10^{-20} \cdot joule$ — The amount of energy (VERY SMALL) in a single photon of light at this wavelength.

What is the energy of a mole of photons at this wavelength (J $mole^{-1}$)?

$E \cdot N = 7.975 \cdot 10^{3} \cdot joule \cdot mole^{-1}$ — Multiply by Avagadro's number

$E \cdot N = 7.975 \cdot kJ \cdot mole^{-1}$ — (Compare this energy to ΔH_{rxn} for a combustion reaction from chapter 6)

Ozone (O_3) in the stratosphere filters out ultraviolet radiation by absorbing light at a wavelength of 250 nm. What is the frequency of this radiation (Hz)? What is the energy of a single photon of this radiation (J)? What is the energy of a mole of photons at this wavelength (J $mole^{-1}$)?

Constants:

$nm := 10^{-9} \cdot m$

Given:

$\lambda := 250 \cdot nm$

What is the frequency of this radiation?

$c = \lambda \cdot \nu$ — Equation that relates the speed (c), wavelength (λ) and frequency (ν) of light.

$\nu := \frac{c}{\lambda}$ — Rearanged to solve for the frequency.

$\nu = 1.199 \cdot 10^{15} \cdot sec^{-1}$

$\nu = 1.199 \cdot 10^{15} \cdot Hz$

What is the energy of a single photon of this radiation (J)

$E := h \cdot \nu$ — Equation that relates the energy (E) and frequency (ν) of radiation using Plank's constant (h)

$E = 7.946 \cdot 10^{-19} \cdot joule$ — The amount of energy (VERY SMALL) in a single photon of light at this wavelength.

What is the energy of a mole of photons at this wavelength (J mole-1)?

$E \cdot N = 4.785 \cdot 10^{5} \cdot joule \cdot mole^{-1}$ — Multiply by Avagadro's number

$E \cdot N = 478.506 \cdot kJ \cdot mole^{-1}$ — (Compare this amout of energy to ΔH_{rxn} for a typical combustion reaction and to the energy of the light for the previous question.)

3. What is the wavelength (nm), frequency (Hz), energy per photon (J) and energy per mole of photons (J $mole^{-1}$) of the radiation produced by the transition of an electron in hydrogen

a. from the n=2 to n=1 level

$n_{initial} := 2 \qquad n_{final} := 1 \qquad R := 1.0974 \cdot 10^{7} \cdot m^{-1}$

The Rydgerg equation from your textbook:

$$\frac{1}{\lambda} = R\left(\frac{1}{n_{final}^{2}} - \frac{1}{n_{initial}^{2}}\right)$$

Substituting in known values for this problem:

$$\frac{1}{\lambda} = 1.0974 \cdot 10^{7} \cdot m^{-1} \cdot \left(\frac{1}{1^{2}} - \frac{1}{2^{2}}\right)$$

Simplifies to:

$$\frac{1}{\lambda} = 1.0974 \cdot 10^{7} \cdot m^{-1} \cdot \left(\frac{1}{1} - \frac{1}{4}\right)$$

$$\frac{1}{\lambda} = 1.0974 \cdot 10^{7} \cdot m^{-1} \cdot (.75)$$

$$\frac{1}{\lambda} = \frac{8230500.}{m}$$

$$\lambda = 1.21499301379017 07065 \cdot 10^{-7} \cdot m$$

This is an example of solving a problem symbolicly with Mathcad. The is series of equations was developed by starting with the top expression. Selecting parts of the equation to calculate (like squaring the two) and then displaying the solution to that step. This allows me to develop the solution the same way you would solve it one step at a time with a piece of paper and a calculator. Notice that this calculation reports the solution to 20 digits, much more that is justified by the significant figures in R.

Alternatively I can rearange the initial equation to make one really large equation and solve in one step, starting from:

$$\frac{1}{\lambda} = R \cdot \left(\frac{1}{n_{final}^{2}} - \frac{1}{n_{initial}^{2}}\right)$$

$$\lambda := -n_{final}^{2} \cdot \frac{n_{initial}^{2}}{\left(-R \cdot n_{initial}^{2} + R \cdot n_{final}^{2}\right)}$$

$$\lambda = 1.215 \cdot 10^{-7} \cdot m$$

Although this is much shorter, all the algebra rearangements are a bit difficult to follow. This is convenient for calculating many problems (since this one equation may now be used with any value of n), but it is more difficult to see how the math is preformed.

I can also really let Mathcad do all the work using numerical techniques where I

Estimates and known values

$n_{initial} = 2$

$n_{final} = 1$

These are the known values of the variables that are required to solve this problem.

$R = 1.097 \cdot 10^{7} \cdot m^{-1}$

$\lambda := 100 \cdot nm$

This is just a guess for the one variable that I do not know the value of. For this technique to work Mathcad needs a "guess" to start with. The more complex the problem the better the guess must be for Mathcad to find a solution.

given

$$\frac{1}{\lambda} = R \cdot \left(\frac{1}{{n_{final}}^{2}} - \frac{1}{{n_{initial}}^{2}} \right)$$

This is where I tell Mathcad how the variables are related. There must be at least one equation for each "unknown".

$\lambda_a := find(\lambda)$

$\lambda_a = 1.215 \cdot 10^{-7} \cdot m$

This tells Mathcad to find the value of λ that fits the relationship given above. This is a very clean way for me to solve problems, but it does not provide all the details about the solutions.

Now that the wavelength of the light is know, the answers to the remaining parts of this question,

$\nu := \frac{c}{\lambda_a}$	$\nu = 2.467 \cdot 10^{15} \cdot Hz$	Frequency
$E := h \cdot \nu$	$E = 1.635 \cdot 10^{-18} \cdot joule$	Energy per photon
	$E \cdot N = 984.587 \cdot kJ \cdot mole^{-1}$	Energy per mole

b. from the n=3 to the n=1 level. $n_{initial} := 3$ $n_{final} := 1$

$$\lambda := -n_{final}^2 \cdot \frac{n_{initial}^2}{\left(-R \cdot n_{initial}^2 + R \cdot n_{final}^2\right)}$$ $\lambda = 1.025 \cdot 10^{-7} \cdot m$

$$\nu := \frac{c}{\lambda}$$ $\nu = 2.924 \cdot 10^{15} \cdot Hz$

$E := h \cdot \nu$ $E = 1.938 \cdot 10^{-18} \cdot joule$

$E \cdot N = 1.167 \cdot 10^{3} \cdot kJ \cdot mole^{-1}$

c. from the n=5 to the n=1 level. $n_{initial} := 5$ $n_{final} := 1$

$$\lambda := -n_{final}^2 \cdot \frac{n_{initial}^2}{\left(-R \cdot n_{initial}^2 + R \cdot n_{final}^2\right)}$$ $\lambda = 9.492 \cdot 10^{-8} \cdot m$

$$\nu := \frac{c}{\lambda}$$ $\nu = 3.158 \cdot 10^{15} \cdot Hz$

$E := h \cdot \nu$ $E = 2.093 \cdot 10^{-18} \cdot joule$

$E \cdot N = 1.26 \cdot 10^{3} \cdot kJ \cdot mole^{-1}$

d. from the n=10 to the n=1 level. $n_{initial} := 10$ $n_{final} := 1$

$$\lambda := -n_{final}^2 \cdot \frac{n_{initial}^2}{\left(-R \cdot n_{initial}^2 + R \cdot n_{final}^2\right)}$$ $\lambda = 9.204 \cdot 10^{-8} \cdot m$

$$\nu := \frac{c}{\lambda}$$ $\nu = 3.257 \cdot 10^{15} \cdot Hz$

$E := h \cdot \nu$ $E = 2.158 \cdot 10^{-18} \cdot joule$

$E \cdot N = 1.3 \cdot 10^{3} \cdot kJ \cdot mole^{-1}$

b. from the n=100 to the n=1 level. $n_{initial} := 100$ $n_{final} := 1$

$$\lambda := -n_{final}^2 \cdot \frac{n_{initial}^2}{\left(-R \cdot n_{initial}^2 + R \cdot n_{final}^2\right)}$$ $\lambda = 9.113 \cdot 10^{-8} \cdot m$

$$\nu := \frac{c}{\lambda}$$ $\nu = 3.29 \cdot 10^{15} \cdot Hz$

$E := h \cdot \nu$ $E = 2.18 \cdot 10^{-18} \cdot joule$

$E \cdot N = 1.313 \cdot 10^{3} \cdot kJ \cdot mole^{-1}$

4. Make a table of the possible quantum numbers for a hydrogen electron that has been excited to a

a. 2s orbital

n = 2	(since this is the **2** s orbital)
l = 0	(since this is an **s** orbital
m_l = 0	(only $\mathbf{m_l}$ possible for an **s** orbital)
m_s = +1/2 or -1/2	(either spin up or spin down is possible)

So the possible combinations are:

2, 0, 0, +1/2
2, 0, 0, -1/2

b. 4p orbital

n = 3	(since this is the **4** p orbital)
l = 1	(since this is a **p** orbital
m_l = -1, 0 or +1	(three possible $\mathbf{m_l}$ for a **p** orbital)
m_s = +1/2 or -1/2	(either spin up or spin down is possible)

So the six possible combinations are:

3, 1, -1, +1/2	3, 1, -1, -1/2
3, 1, 0, +1/2	3, 1, 0, -1/2
3, 1, 1, +1/2	3, 1, 1, -1/2

c. 5d orbital

n = 5	(since this is the **5** d orbital)
l = 2	(since this is a **d** orbital
m_l = -2, -1, 0, +1, or +2	(five possible $\mathbf{m_l}$ for a **d** orbital)
m_s = +1/2 or -1/2	(either spin up or spin down is possible)

So the ten possible combinations are:

5, 2, -2, +1/2	5, 2, -2, -1/2
5, 2, -1, +1/2	5, 2, -1, -1/2
5, 2, 0, +1/2	5, 2, 0, -1/2
5, 2, 1, +1/2	5, 2, 1, -1/2
5, 2, 2, +1/2	5, 2, 2, -1/2

c. 6f orbital

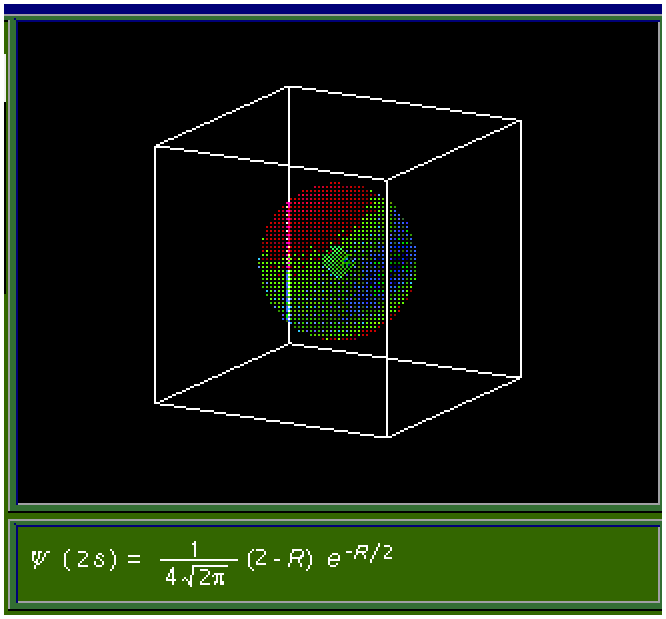
n = 6	(since this is the **6** f orbital)
l = 3	(since this is a **f** orbital
m_l = -3, -2, -1, 0, +1, +2, or +3	(five possible $\mathbf{m_l}$ for a **d** orbital)
m_s = +1/2 or -1/2	(either spin up or down possible)

So the fourteen possible combinations are:

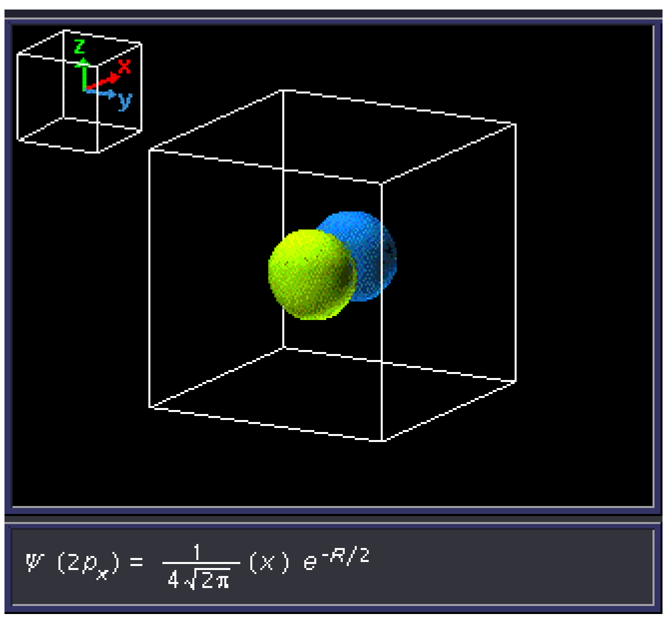
6, 3, -3, +1/2	6, 3, -3, -1/2
6, 3, -2, +1/2	6, 3, -2, -1/2
6, 3, -1, +1/2	6, 3, -1, -1/2
6, 3, 0, +1/2	6, 3, 0, -1/2
6, 3, 1, +1/2	6, 3, 1, -1/2
6, 3, 2, +1/2	6, 3, 2, -1/2
6, 3, 3, +1/2	6, 3, 3, -1/2

5. Draw diagrams of the following orbitals, (These figures are from *Atomic Orbitals CD*, release 1.0 by Yue-Ling Wong.

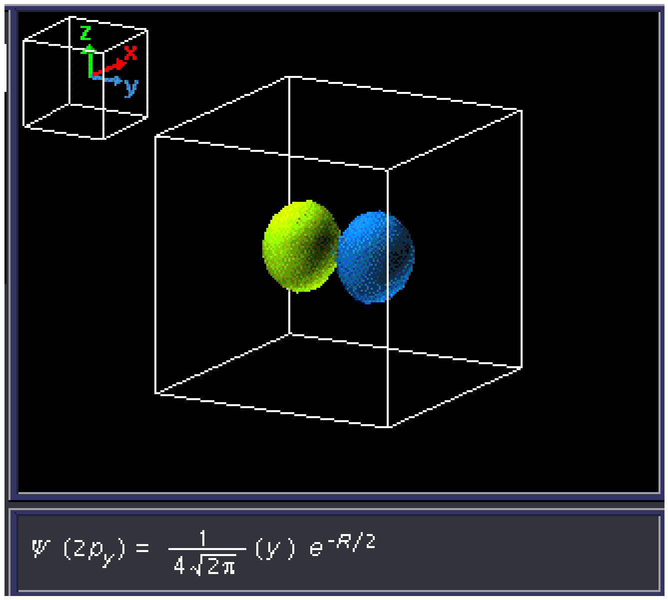
a. 1s



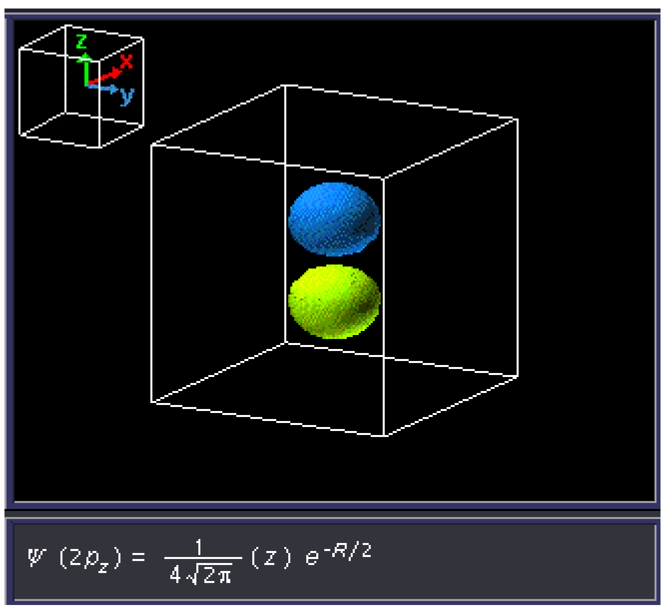
b. $2p_x$



c. $2p_y$



d. $2p_z$



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