**General Chemistry C, Fall 2023**
**Problem Set 1**

- *Due date: 2023/09/20 10:00 AM.*
- *Write down how you calculate the answer step-by-step (don't forget about the units).*
- *Please upload a PDF file containing your answers to NTU COOL.*

1. (4 pt) The EUV lithography systems used in the semiconductor device fabrication process output electromagnetic radiation with 13.5 nm wavelength. (a) What is the frequency of this radiation? (b) Assuming the dose energy required per exposure is 470 mJ, how many EUV photons are needed for each exposure?

   (a)
   $c = f\lambda = 2.99 \times 10^{8}\ ({}^{m}/_{s}) = f \times 13.5 \times 10^{-9}\ (m)$
   $f\ = 0.22148 \times 10^{17}\ (s^{-1}) = 2.21 \times 10^{16}\ (s^{-1})$
   1pt for c = f x $\lambda$
   0.5 pt for correct s.f.
   0.5 pt for unit

   (b)
   $1\ (Joule) = 6.24 \times 10^{18}\ (eV)$
   $470\ (mJ) = 2.932 \times 10^{18}\ (eV)$
   $\#\ of\ photon \times \frac{1240\ ({}^{nm}/_{eV})}{13.5\ (nm)} = 2.932 \times 10^{18}\ (eV)$
   $\#\ of\ photon = 3.19 \times 10^{16}$
   1 pt for energy conversion (not necessary to convert from joule to eV)
   0.5 pt for stating the equation correctly
   0.5 pt for correct s.f.

2. (6 pt) Vibranium is a fictional metal in the Marvel Comic series. Assuming the work function of vibranium is 2.63 eV (1 eV = 1.602 x $10^{-19}$ J), (a) calculate the minimum frequency of light required to eject electrons from a clean vibranium surface. (b) If vibranium is illuminated by 365 nm light, what is the ejected electrons' kinetic energy (in J)?

(a)

$E_{photon} = E_{kinetic} + \varphi = 0 + 2.63\ (eV)$

$E_{photon} = 2.63\ (eV) \times 1.602 \times 10^{-19}\ \left({}^{J}/_{eV}\right) = h\nu = 6.626 \times 10^{-34}\ (Js) \times \nu$

$\nu = 6.36 \times 10^{14} (s^{-1})$

1 pt for correct photovoltaic relation
1 pt for correct conversion of energy
0.5 pt for correct s.f.
0.5 pt for correct unit

(b)

$365\ (nm) = 3.40\ (eV)$

$E_{photon} = 3.40\ (eV) = E_{kinetic} + 2.63\ (eV)$

$E_{kinetic} = 0.770\ (eV) = 1.23 \times 10^{-19}\ (J)$

1 pt for correct conversion from wavelength to energy
1 pt for stating kinetic energy = light energy - work function
0.5 pt for correct s.f.
0.5 pt for correct unit

3. (4 pt) In an electron microscope, electrons are accelerated by passing them through a voltage difference. The kinetic energy thus acquired by the electrons is equal to the voltage times the charge of the electron. Thus, a voltage difference of 1 volt (V) imparts a kinetic energy of 1.602 x $10^{-19}$ J. Calculate the de Broglie wavelength (in pm) associated with electrons accelerated by 1.50 x $10^4$ V.

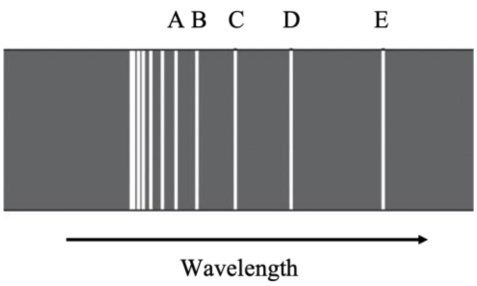
$E_{kinetic} = \frac{P^2}{2m_e} = 1.602 \times 10^{-19} (Q) \times 1.50 \times 10^4\ (V) = 2.40 \times 10^{-15}\ (J)$

$P = 6.62 \times 10^{-23} (Kg \cdot {}^{m}/_{s})$

$\lambda = \frac{h\ (Js)}{P\ (Kg \cdot {}^{m}/_{s})} = \frac{6.626 \times 10^{-34} (Js)}{6.62 \times 10^{-23} (Kg \cdot {}^{m}/_{s})} = 1.00 \times 10^{-11} (m) = 10.0\ (pm)$

1 pt for matter-wave equation
1 pt for correct conversion of kinetic energy
1 pt for correctly giving the relation between wavelength and momentum
0.5 pt for correct s.f.
0.5 pt for correct unit

4. (6 pt) The figure to the right represents the emission spectrum for a one-electron atom/ion in the gas phase. All the lines shown are resulted from electronic transitions from excited states to the n=3 state. (a) Describe the electronic transitions corresponding to lines A and E. (b) If the wavelength of line E is 208. nm, what is the atomic number of this atom/ion? (c) Calculate the wavelength of line A to 3 significant figures.




(a)
A: $n = 8 \rightarrow n = 3$
B: $n = 7 \rightarrow n = 3$
C: $n = 6 \rightarrow n = 3$
D: $n = 5 \rightarrow n = 3$
E: $n = 4 \rightarrow n = 3$
1 pt each line

(b)
For a one-electron system atom/ion system, $E_n = R_H Z^2[\frac{1}{n_f^2} - \frac{1}{n_i^2}]$, where Z is nuclear charge, $R_H$ is Rydberg constant $= 1.097 \times 10^7\ m^{-1}$, f is the final state, and i is the initial state.

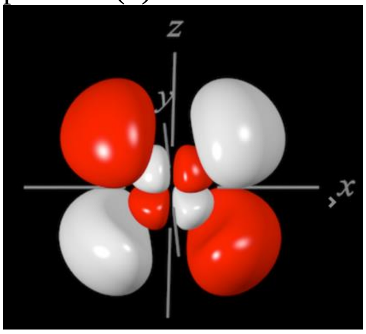
Line E is corresponding to $n = 4 \rightarrow n = 3$
$Z^2 = \frac{1}{\lambda} \times \frac{1}{R_H[\frac{1}{9} - \frac{1}{16}]} = 1$ , so $Z = 3$

2 pt for correct relation of Bohr's atomic model
1 pt for correct answer

(c) Line A is corresponding to $n = 8 \rightarrow n = 3$
By using $\frac{1}{\lambda} = R_H Z^2[\frac{1}{n_f^2} - \frac{1}{n_i^2}]$, we can obtain $1.06 \times 10^{-7} m$
Also, one can use $\lambda$ of line E to get that of line A:
$208\ nm \times \left[\frac{1}{9} - \frac{1}{16}\right] \div \left[\frac{1}{9} - \frac{1}{64}\right] = 106(nm) = 1.06 \times 10^{-7}(m)$

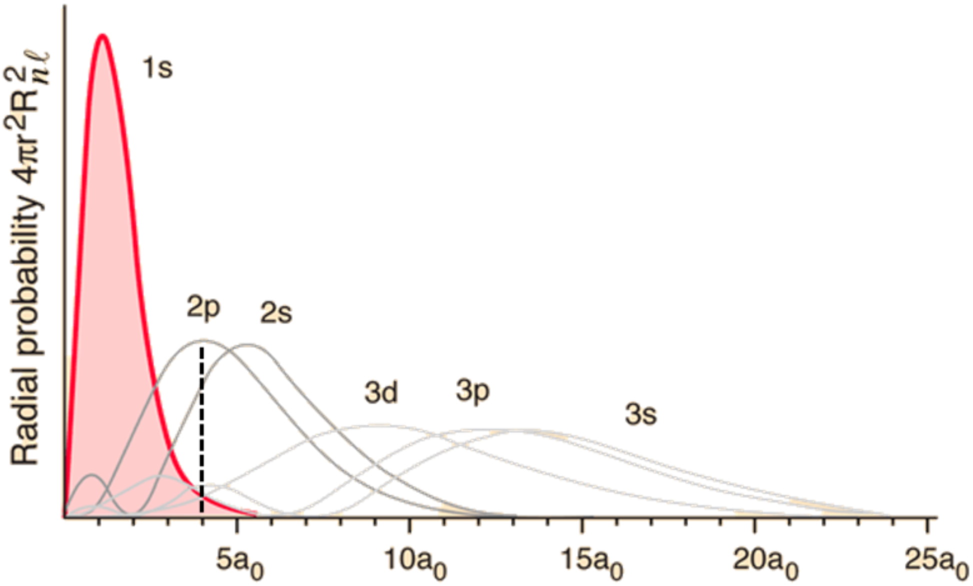
0.5 pt for correct answer
0.5 pt for correct s.f.

5. (4 pt) For a particle-in-a-1D-box system, the n=4 → n=2 transition emits a 415 nm photon. To which wavelength (in nm) does the n=3 → n=1 transition correspond?
From particle in a 1-D box, we know that allowed energy ($E_n$) and the allowed energy transfer between each state ($\Delta E$), furthermore, we can convert the energy of light into wavelength as below:
$E_n = \frac{n^2h^2}{8mL^2}, n = 1,2,3, \ldots$
$\Delta E = E_f - E_i = \frac{h^2}{8mL^2}(f^2 - i^2)$
$\frac{1}{\lambda} = \frac{\Delta E}{hc} = \frac{h}{8mL^2c}(f^2 - i^2)$
Where, L is the size of the particle, which isn't important in the case.
For the transition of $n = 4 \rightarrow n = 2$:
$\frac{1}{\lambda_{4\rightarrow 2}} = \frac{1}{415} = \frac{h}{8mL^2c}(4^2 - 2^2)$
For the transition of $n = 3 \rightarrow n = 1$:
$\frac{1}{\lambda_{3\rightarrow 1}} = \frac{h}{8mL^2c}(3^2 - 1^2)$
We can divide the 2 equations to eliminate all other parameters that we don't want to get this equation:
$\frac{\lambda_{3\rightarrow 1}}{\lambda_{4\rightarrow 2}} = \frac{\lambda_{3\rightarrow 1}}{415} = \frac{(4^2-2^2)}{(3^2-1^2)} = \frac{3}{2}$
$\lambda_{3\rightarrow 1} = 4.15 \times 10^{-7}(m) \times \frac{3}{2} = 6.23 \times 10^{-7}(m) = 623(nm)$
6. (6 pt) Give the values of the quantum numbers (n, l, $m_l$) associated with the following orbitals: (a) 2p, (b) 5d, and (c) 4p.
(a) 2p
$n = 2;\ l = 1; m_l = 0, \pm 1$
(b) 5d
$n = 5;\ l = 2; m_l = 0, \pm 1, \pm 2$
(c) 4p
$n = 4;\ l = 1; m_l = 0, \pm 1$
2 pt each answer, get only 1pt if not correctly give each $m_l$
7. (4 pt) (a) How many angular nodal planes and radial nodal planes are in the following picture? (b) Which atomic orbital is this?




(a) There are two angular nodal planes (1pt) and one radial nodal plane (1pt) in the picture.
(b) Two angular nodal planes indicate that it is a d orbital.
One radial nodal plane shows that its principal quantum number is 4. (4d orbital)
The orbital lies in the xz plane, which means it is a 4dxz orbital. 4d(1pt)xz(1pt)

8. (6 pt) The radial wavefunction of 2p orbital is $R_{nl}(r) = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$, in which Z is the nuclear charge and $a_0$ is the Bohr radius. Prove that the most probable distance to find a 2p electron in hydrogen is at $r = 4a_0$.




Radial probability $P_{nl}(r) = 4\pi r^2 R_{nl}^2(r)$

$= 4\pi r^2\left[\frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{\frac{2}{3}}\left(\frac{Zr}{a_0}\right)e^{-\frac{Zr}{2a_0}}\right]^2 = \left[\frac{4\pi}{24}\left(\frac{Z}{a_0}\right)^5\right]r^4 e^{-\frac{Zr}{a_0}} - (1pt)$

The most probable distance is the distance $r_{probable}$ where the probability reaches the maximum. Thus, we take the first derivative for $P_{nl}$.

$\frac{dP_{nl}(r)}{dr} = \left[\frac{4\pi}{24}\left(\frac{Z}{a_0}\right)^5\right][4r^3 + r^4\left(-\frac{Z}{a_0}\right)]e^{-\frac{Zr}{a_0}} = 0 - (3pt)$

$=> \left[4r^3 + r^4\left(-\frac{Z}{a_0}\right)\right]e^{-\frac{Zr}{a_0}} = 0 => 4 + r\left(-\frac{Z}{a_0}\right) = 0 => r_{probable} = \frac{4a_0}{Z}$

For hydrogen atom, Z =1. Therefore, we can get $r_{probable} = 4a_0$. (2pt)

The second order derivative should also be considered to prove the function reaches its maximum at $r = 4a_0$, that is, $\frac{d^2P_{nl}(r)}{d^2r} < 0$.

9. (10 pt) (a) Write down the ground state electron configurations of the following atoms and ions: N, $S^{2-}$, $Na^{+}$, $Ti^{3+}$, $Fe^{2+}$. (b) Indicate how many unpaired electrons are in these atoms and ions.

(a)
N: $1s^2 2s^2 2p^3$ (1pt)
S: $1s^2 2s^2 2p^6 3s^2 3p^4 \rightarrow S^{2-}$: $1s^2 2s^2 2p^6 3s^2 3p^6$ (1pt)
Na: $1s^2 2s^2 2p^6 3s^1 \rightarrow Na^{+}$: $1s^2 2s^2 2p^6$ (1pt)
Ti: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^2 \rightarrow Ti^{3+}$: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^1$ (1pt)
Fe: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6 \rightarrow Fe^{2+}$: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$ (1pt)

(b)
N: 3 unpaired electrons (1pt)
$S^{2-}$: 0 unpaired electron (1pt)
$Na^{+}$: 0 unpaired electron (1pt)
$Ti^{3+}$: 1 unpaired electron (1pt)
$Fe^{2+}$: 4 unpaired electron (1pt)