1. Give a short answer or explanation for the following questions.
(a) Why is an atom of Br bigger than an atom of Cl?

(b) Explain what Z* is and how it can be estimated by Slater's Rules.

(c) Write equations for the first three ionization energies of Calcium.

\[
\begin{align*}
\text{Ca}(g) & \rightarrow \text{Ca}^{+} + \text{e}^{-} \quad \text{IE}_1 \\
\text{Ca}^{+}(g) & \rightarrow \text{Ca}^{2+} + \text{e}^{-} \quad \text{IE}_2 \\
\text{Ca}^{2+}(g) & \rightarrow \text{Ca}^{3+} + \text{e}^{-} \quad \text{IE}_3
\end{align*}
\]

The first three ionization energies for calcium are
\[
\text{IE}_1 = 589.8 \text{ kJ/mol}, \quad \text{IE}_2 = 1,145.4 \text{ kJ/mol}, \quad \text{IE}_3 = 4,912.0 \text{ kJ/mol}
\]

(d) Explain why the ionization energy increases in order \( \text{IE}_1 < \text{IE}_2 < \text{IE}_3 \).

(e) \( \text{IE}_2 \) is 94% larger than \( \text{IE}_1 \), but \( \text{IE}_3 \) is 328% larger that \( \text{IE}_2 \).

(f) Identify the following terms in the above equation.

\[
\Psi_{n,l,m}(r, \theta, \phi) = R_{n}(r) \cdot Y_{l,m}(\theta, \phi)
\]

\( R_{n}(r) \) a solution to Schrödinger's Eqn. \quad \text{radial part}

\( Y_{l,m}(\theta, \phi) \) \text{angular part} \quad (r, \theta, \phi) \text{spherical polar coordinates}

\( n, l, m \) quantum numbers

(g) Why was it necessary to replace Bohr’s model of the atom?
2. (a) Sketch the wavefunction, \( \psi \), for a particle in a box of length \( a \) for energy level \( n = 4 \).

(b) Sketch the probability function, \( \psi^2 \), for a particle in a box of length \( a \) for energy level \( n = 3 \).

(c) The energy levels for the particle in a box are quantized. Explain what this means.

Only certain values are allowed for the energy. These are labeled by \( n \), the quantum number,
5. Write the electron configuration of the following atoms or ions. You may use the noble gas short hand notation. (1 pt each)

(a) Fe^{2+} \[ \text{Ar} ] 3d^5 \ (8 - 3 = 5) \quad \text{(b) Cl} \ [\text{Ne}] 3s^2 3p^5

(c) Se^{2-} \[ \text{Kr} \]

(d) Se^{3-} \[ \text{Kr} \]

(e) U\ [\text{Xe}] 7s^2 6d^{15}f^3 \ or \ 7s^5 5f^4

(f) Ag\ [\text{Kr}] 5s^2 4d^9 \ or \ 5s^4 4d^{10}

Circle the correct species with the given property in each set (g) through (n). (2 pt each)

(g) Largest radii \[ F^- > Na^+ > Li^+ \]

(h) Largest radii \[ Mg^{2+} \quad Mg^+ \quad Mg \]

(i) Largest atomic radii \[ N \quad P \quad As \]

(j) Largest atomic radii \[ Br \quad Cu \quad Se \]

(k) Most electronegative \[ N \quad P \quad O \]

(l) Greatest ionization energy \[ S^{2-} \quad S^+ \quad S \]

(m) Greatest 1st ionization energy \[ N \quad P \quad As \]

(n) Greatest 1st ionization energy \[ N \quad As \quad P \]

(o) In general ionization energy increases across a period, however the first ionization energy of O is actually lower than that of N. Explain why this is so. (3 pts)

N \[ 1s^2 2s^2 2p^3 \] = 1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1

O \[ 1s^2 2s^2 2p^4 \] = 1s^2 2s^2 2p_x^2 2p_y^1 2p_z^2

Removing e^- from O also removes the e^- e^- repulsion of the doubly occupied orbital 2p_x^2. This makes IE_1 less than expected.
4. For (a)-(c) include a coordinate system and label the axes for each orbital.

(a) Draw the shape of **angular** part of the wavefunction, \( Y(\theta,\phi) \), of the hydrogen atom for an s orbital

![Sphere](image)

(b) Draw the shape of the **angular** part of the wavefunction, \( Y(\theta,\phi) \), of the hydrogen atom for the \( p_y \) orbital

![Along y axis](image)

(c) Draw the shape of the **angular** part of the wavefunction, \( Y(\theta,\phi) \), of the hydrogen atom for the \( dxz \) orbital

![In xz plane, between \( \pm x \) and \( \pm z \) axes](image)

(d) Draw the shape of the **angular** part of the wavefunction, \( Y(\theta,\phi) \), of the hydrogen atom for the \( dz^2 \) orbital

![Image](image)
4. Consider the $4p_z$ hydrogen-like orbitals and consider a hydrogen atom. Radial nodes occur at $5.5 \ a_0$ and $14.5 \ a_0$.

(a) Sketch the radial function, $R(r)$

(b) Sketch the radial probability function, $4\pi r^2 R^2(r)$.

(c) Contour maps of the electron density.
3. Oops! Someone forgot to label the following orbitals. Using what you know about the number of nodes and the form of the functions place the labels under the appropriate graphs.

Labels to use
- \( R_{n,l}(r) \) for the 3s orbital
- \( 4\pi^2 R_{n,l}^2(r) \) for the 4s orbital
- \( R_{n,l}(r) \) for the 4s orbital
- \( 4\pi^2 R_{n,l}^2(r) \) for the 3d orbital
- \( R_{n,l}(r) \) for the 2p orbital
- \( 4\pi^2 R_{n,l}^2(r) \) for the 4p orbital
- \( R_{n,l}(r) \) for the 4d orbital
- \( 4\pi^2 R_{n,l}^2(r) \) for the 1s orbital

When I gave the test I cut out the figures of the above functions and mixed them up. They are in the book or handout.

**Guidelines**
1. \( R_{n,l}(r) \) may be (-)
2. \( 4\pi r^2 \) \( R_{n,l}^2(r) \) is always (+)
3. The first time an orbital appears it has no nodes: 1s, 2p, 3d, 4f;
   the second time 1 radial node: 2s, 3s, 4d, 5f, etc.
4. All \( 4\pi r^2 \) \( R_{n,l} \) functions are = 0 at \( r = 0 \)
5. \( R_{n,l}(r) \) in 5 orbital ≠ 0 at \( r = 0 \)
   \( R_{n,l}(r) \) p, d, f, orbital = 0 at \( r = 0 \)

Rough sketch:
- \( R_{n,l} 3s \leftarrow 1 \) radial node doesn't start at zero
- \( R_{n,l} 2p \leftarrow \) zero radial nodes start at zero
- \( R_{n,l} 4d \leftarrow 1 \) radial node
- \( R_{n,l} 4s \leftarrow 2 \) radial nodes doesn't start at zero
6. The energy of a transition within a hydrogen atom are given by the following equation:

\[ \Delta E = -2.1781 \times 10^{-18} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \text{ Note fall 2003 we use -13.6 eV} \]

(a) Calculate the wavelength of light associated with transition between level \( n = 7 \) to \( n = 3 \) for \( \Delta E = -2.178 \times 10^{-18} \) J.

\[ \Delta E = -2.1781 \times 10^{-18} \left( \frac{1}{3^2} - \frac{1}{7^2} \right) \nu \cdot \frac{n_f}{n_i} = -2.1781 \times 10^{-18} \left( 9.070 \times 10^{-2} \right) \]

\[ \Delta E = -1.976 \times 10^{-19} \text{ J} \]

\[ \Delta E = h \nu \]

\[ \lambda = \frac{6.626 \times 10^{-34} \text{ J s} \times 2.998 \times 10^8 \text{m/s}}{1.976 \times 10^{-19} \text{ J}} \]

\[ \lambda = \frac{h \nu}{\Delta E} \]

\[ \lambda = 1.006 \times 10^{-6} \text{ m} \times \frac{1 \text{ nm}}{10^{-9} \text{ m}} = 1005 \text{ nm} \]

(b) Is this light absorbed or emitted from the atom in this transition?

\((-) \text{ means exothermic, so light is emitted.}\)