Your name:	______________________
ID number:	______________________

<u>Section 1 (9 am)</u>

Problem	Maximum number of points	Points earned
1	30	
2	30	
3	30	
4	30	
5	30	
Total	150	

The exam is open book and open notes. However, please refrain from talking to each other, and using internet, or cell phones. You may use a calculator. All necessary constants are provided in the formula sheet, for your convenience. Report your answers in SI units unless otherwise specified.

Show all your calculations/work to receive full credit!

Make sure to CLEARLY write (print) your name and ID number (as shown on your student ID) at the top of the front page. Anything written outside the box will **NOT** be graded.

Good luck!

1) (30pts) Brian used a gaseous Li^{2+} sample in its fourth excited state to conduct an atomic emission spectrum experiment.
   a) (10pts) Brian observed multiple bright lines on a dark background in their final emission spectrum. Explain the physical meaning of the bright lines on the spectrum. Then use an energy level diagram to predict how many lines should Brian observe?
   b) (10pts) Calculate the wavelength of the first line (low wavelength lines appear first) on the emission spectrum.
   c) (10pts) Estimate the energy required to form Li^{3+} from Li^{2+} (second excited state). What type of EM radiation is needed for this process to take place?

2) (30pts) A few months ago, scientists discovered a new method to deconstruct waste polyethylene using Hoveyda-Grubbs Catalyst, 2nd Generation (**HG2**).
   a) (5pts) The chemical formula of **HG2** used is $C_{29}H_{33}X_2Y_2ORu$. X is a halogen in period 3, and Y has two less proton than Fluorine. What is the atomic number of X and Y?
   b) (5pts) Calculate the molecular weight of **HG2**.
   c) (10pts) Ru exists in multiple stable isotopes, with mass number 99, 100, 101, 102, and 104. List the number of protons and neutrons in each stable isotope.
   d) (10pts) Ashley wish to conduct molecular dynamics calculations to study the polyethylene decomposition reaction in Xylene (C_8H_{10}). They created a spherical solvent box with radius r = 100 Å. Given the density of Xylene is 0.861 g/ml, estimate the number of molecules of Xylene in the solvent box.

3) (30 pts) Claire, a young chemist, assembled a photoelectric experiment as they learned in Chem 20A class. With a gold (Au, Φ = 5.30 eV) photocathode, they initially used a yellow laser with wavelength λ=600 nm. Interestingly, Claire observed no photoelectron ejection and cannot understand why.

$$1\ eV = 1.602 \times 10^{-19}\ J$$

a) (10pts) Briefly explain why photoelectron ejection is not observed. Justify your answer with calculations.

b) (5pts) Can you suggest a maximum wavelength required to obtain photoelectron ejection from the gold photocathode?

c) (15pts) Claire switched to a UV laser with wavelength λ=160 nm. Calculate the De Broglie wavelength of the ejected photoelectrons. Assume ejected photoelectrons all have maximum kinetic energy.

4) (30 pts) David would like to solve the Schrödinger equation for the following 1D-particle in a box problem. Given the Hamiltonian operator of this particle ☺ is:

$$\mathcal{H} = -\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2} + U(x)$$

This 1D box has the following set up:

$$U(x) = \begin{cases} \infty \;\; for\ x \leq 0\ or\ x \geq 4L\ ; & outside\ the\ box \\ \pi \;\; for\ 0 < x < 4L; & inside\ the\ box \end{cases}$$

a) (10pts) Given that the general form of the wavefunction can be:

$$\Psi(x) = A\sin(kx)$$
$$\Psi(x) = A\cos(kx)$$
$$\Psi(x) = Ae^{kx}$$

Choose the correct general form of the 1D PIB wavefunction and solve for coefficient k.

b) (15pts) Solve the allowed energy levels of ☺. The mass of ☺ is m. You can express your energy in quantum number n and constants h, π, m and L.

$$magic\ calculus\text{:}\ \frac{d^2}{dx^2}A \times sin(kx) = -A \times k^2 \sin(kx)$$

c) (5 pts) What is the probability of finding ☺ in 4th excited state in region (L, 2L)? You only need to set up the integral.

5) (30pts) Hydrogenic orbitals ($\Psi_{nlm}(r, \theta, \phi)$) can be solved analytically (to an exact mathematic equation).

   a) (5pts) Write all possible quantum number combinations and their conventional names for n = 3. You do not need to specify the conventional name corresponding to the magnetic quantum number.
   b) (5pts) Briefly explain why there exist three p and five d atomic orbitals.
   c) (10pts) The radial wavefunction of Be^{3+} **4p** atomic orbital is given in the following equation:

$$R_{4p} = \frac{1}{32\sqrt{15}}(Z^{\frac{3}{2}})\frac{2Zr}{n}(20 - 10\frac{2Zr}{n} + \frac{4Z^2r^2}{n^2})e^{-\frac{Zr}{n}}$$

   At what distances r ($r \leq 10a_0$) you expect zero probability in finding the Be^{3+} *4p* electron? (Assume the unit of r is Bohr radius a_0)

   d) (10pts) sketch the Be^{3+} **4p$_z$** atomic orbital. Label positions of the radial nodes.