General and Structural Chemistry
Assignment-1

Full Marks: 100

Q1. Write the set of four quantum numbers for the "last" electron in the atom, V. [2]

Q2. Write down the quantum numbers defined by the angular wavefunction for a dz^2 orbital. [2]

Q.3. Write down the respective eigen value for the following operation on the Spherical Harmonics eigenfunction, $Y_l^m(\theta,\varphi)$: [2]

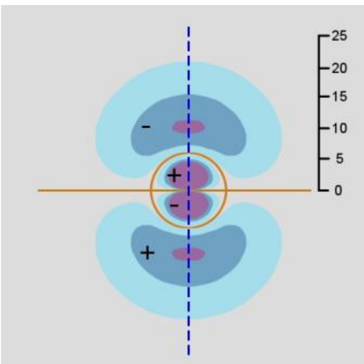
$$-i\hbar\,\frac{\partial}{\partial\phi}Y_\ell^m(\theta,\phi)$$

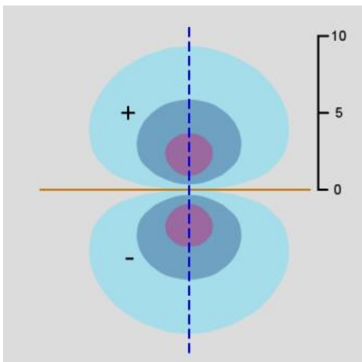
Q4. What is meant by degenerate energy levels? Give an example. [3]

Q5. (a) Write down the expression for the wavefunction [$\psi_{2,1,0}(r,\theta,\varphi)$] for hydrogen-like atoms with atomic number Z. Define the terms. [4]
(b) Write the expression for its radial distribution function. [6]
(c) Using this density probability expression (radial distribution function), find out the position of nodes and the expected radial distance. [6+6]
(d) Write the expression for its $Y_{1,0}$. [3]
(e) Using the appropriate mathematical expression, determine its nodal plane. [4]

Q6. Calculations show that the 4*s*-obital has higher energy than a 3d-orbital of the same atom. However, according to Aufbau principle, 4s-orbital gets filled up first in 3d-transion elements. How can one justify the above observation? [4]

Q7. The following plots show the orbital contour diagrams of some orbitals of a hydrogen-like atom. **Identify** each of them and **explain** how you arrived at your decision. An electron will be in the most-likely-10% (purple) regions 10% of the time, and it will be in the most-likely-50% regions (including the most-likely-10% regions, dark blue and purple) 50% of the time. [3+3]



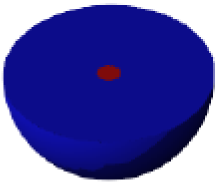


Q.8. Given that the spherical representation of the d_{x2-y2} orbital is $r^2 sin^2(\theta) cos(2\phi)$, show that this matches the label for the orbital, x^2-y^2. Hint: cos(2x)=cos2(x)−sin2(x) [3]

Q.9. Write down the unique magnetic quantum numbers of the wavefunctions corresponding to p_x, p_y, and p_z-orbitals. [3]

Q.10. Write down the electronic configuration for the ground state boron atom. Into how many distinct beams will a beam of boron atoms be split when it is passed through an atomic beam apparatus with an inhomogeneous magnetic field directed perpendicular to the direction of travel of the atoms? How does it differ from an atom with electronic configuration: $1s^2 2s^1$?

Q.11. Consider the orbitals (a cross-section diagram) shown here.



(a) What is the maximum number of electrons contained in an orbital of the above type? [2]

(b) How many orbitals of this type are found in a shell with n = 4? [2]

(c) What are the possible l and m_l values for an orbital of the above type? [2]

Q.12. Suppose when a beam of hydrogen atoms (with l = 0) is passed through an atomic beam apparatus, the magnetic field causes the beam to split into four (4) separate beams. Excepting this, if all of the laws of quantum mechanics applied here, (a) what is the value of the spin quantum number s in the above case and what are the possible values for the spin magnetic quantum number m_s? (b) How many electrons may occupy an orbital with given values of n, l and m_l in the above case? (c) State how many elements would appear in the first, second, third and fourth rows of the new periodic table of the elements if the above case is true. Give reasons. (d) What would be the ground state configurations of the elements with atomic numbers Z = 7 and 10 and what would their valences be? (e) Which element would be the first of the noble gases in such a case? [4+2+16+8+4]