Chemistry 448 Test 1 Name:_______________
Fall 2025

Very Short Answer Questions: (3 points each)

1. What is the electron configuration of Te^{4+}? [Kr] $5s^2\ 4d^{10}$

2. The size of atoms decreases moving right across the periodic table.

3. The probability of finding an electron at a given point equals ψ^2.

4. Ionization energy - The energy required to remove an electron from a gas phase atom or ion.

5. The first ionization energy of phosphorus is somewhat larger than expected when compared with where it is expected to be found.

6. The angular wave function is independent of energy (the principle quantum number).

7. The absence of an S_n axis defines a molecule as being chiral (dissymmetric).

8. Is it possible for a molecule belonging to a dihedral point group (e.g. D_n, D_{nh}, or D_{nd}) to exhibit a dipole moment? No

9. For BF_3, what symmetry element is obtained if the following multiplication is performed: $C_2 \otimes C_3$? σ_v (Your answer should be neither C_2 nor C_3.)

10. Boron is the one element from Groups I-IIIA that is a semiconductor when pure.

Discussion Questions: (You must show your work to receive credit!)

1. Why is quantization a consequence of the Schrödinger equation? (Answer with respect to the particle-in-a-box problem.) (10 points)

   If the boundary condition for the particle-in-a-box is accepted, then the resultant solution is a sine function equal to zero at the boundaries. This can only occur for whole number multiples of π. Thus, only certain solutions are possible to the particle-in-a-box which is the definition of quantization.

2. How can 3 of the following 4 be isolated from their naturally occurring sources: Al, He, Mg, Na? (9 points)

   See handouts.

3. Which of the following is more stable and why? (10 points)

   (a) **Co^{2+}** or V^{2+} - Effective nuclear charge increases in moving from left to right in any row because the newly added electrons don't shield as well as core electrons. As a result, the electrons on cobalt are drawn closer to the nucleus than on vanadium. That these are ions doesn't matter since the charges are the same.

(b) Ta^{2+} or <u>**V^{2+}**</u> - The valence electrons on vanadium and tantalum lie in the n = 6 and n = 4 shells, respectively. A higher principal q.n. means the energy of electrons in those orbitals is higher, resulting in them residing further from the nucleus, making the radius larger.

4. There are two types of nodes. What are they and what physical significance do they have if any? (i.e. Would we notice a difference in atoms if all nodes were removed? What would the difference(s) be?) (10 points)

   Angular and radial nodes. Angular nodes give rise to the shape of the orbital. Recall that nodes are regions of zero electron density and regions near nodes have very low electron densities. The relative volumes affected significantly by nodal surfaces is greatest near nuclei. That is, percent of total volume affected by nodes is greater near the nucleus than far from it. The result is that electrons are pushed away from nuclei. Presumably removing nodes would allow electrons to spend more time closer to the nucleus and so electrostatic attraction would increase. This would result in higher ionization energies and electron affinities and smaller atoms.

5. Give point groups for each of the following (no work required): (16 points)

B_2H_6: D_{2h}	C_6H_{12} (Chair conformation): D_{3d}
the letter "W": C_{2v}	*cis*-$Cr(CO)_4(PH_3)_2$: C_{2v}

6. As you know the H^+ ion is easily generated in aqueous solution. In spite of this, the ionization energy of a hydrogen atom is not only the largest of the Group IA elements, it is largest by a lot more than is initially expected. Why? (5 points)

   The hydrogen atom is unique among the elements in that it has no core. A result is that its valence electron is not shielded. Thus, it is the only element for which $Z = Z_{eff}$. experienced by the electron. To get the high ionization energy, the close approach of the electron must be considered as well. In hydrogen, the valence electron has its most probable radius much smaller that that of even lithium, thus providing for a high ionization energy.

7. Using the character table below, generate the reducible representation for CH_4 (Hint: $\Gamma(C_3) = 0$) How many total vibrations occur in a methane molecule and what are they? What are the C-H stretches? (10 points)

	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_v$
Γ(total)	15	0	-1	-1	3
Γ(C-H)	4	1	0	0	2

<u>Total</u>

$A_1 = 1/24[(15)(1)(1) + (0)(8)(1) + (-1)(3)(1) + (-1)(6)(1) + (3)(6)(1)] = 1$

$E = 1/24[(15)(1)(2) + (0)(8)(-1) + (-1)(3)(2) + (-1)(6)(0) + (3)(6)(0)] = 1$

$T_1 = 1/24[(15)(1)(3) + (0)(8)(0) + (-1)(3)(-1) + (-1)(6)(1) + (3)(6)(-1)] = 1$

$T_2 = 1/24[(15)(1)(3) + (0)(8)(0) + (-1)(3)(-1) + (-1)(6)(-1) + (3)(6)(1)] = 3$

Translations and vibrations are represented by T_2 and T_1, respectively and must be removed from the total. The resulting vibrations are A_1, E, and 2 T_2.

C-H Stretches

$A_1 = 1/24[(4)(1)(1) + (1)(8)(1) + (0)(3)(1) + (0)(6)(1) + (2)(6)(1)] = 1$

$T_2 = 1/24[(4)(1)(3) + (1)(8)(0) + (0)(3)(-1) + (0)(6)(-1) + (2)(6)(1)] = 1$

Thus C-H stretches are represented by an A_1 and T_2 mode. (Note: This is a subset of part a.)