2018 Fall Semester Quiz 2
For General Chemistry I (CH101)

Date: October 1 (Mon), Time: 19:00 ~ 19:45

Professor Name	Class	Student I.D. Number	Name

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1. (Total 10 pts, each 2 pts for a right answer, - 2 pt for a wrong answer, 0 pt for no answer) **Read the following statements or equations, and verify whether these are "TRUE (T)" or "FALSE (F)". (2 pts for a right answer, -2 pts for a wrong answer, 0 pt for no answer)**

(a) The energy of a one-electron atom depends only on the principal quantum number n, because the potential energy depends only on the radial distance.

Answer: _____**True**_____

(b) Solutions of the Schrodinger equation for a one-electron atom or ion with atomic number Z exist only for particular values of the energy:

$$\mathrm{E_n} = \frac{Z^2 e^4 m_e}{8\epsilon_0^2 n^2 h^2} \qquad \boldsymbol{n = 1, 2, 3, \ldots} \rightarrow \mathrm{E_n} = -\frac{Z^2 e^4 m_e}{8\epsilon_0^2 n^2 h^2}$$

Answer: _____**False**_____

(c) S^- and Ar^+ are diamagnetic. → Paramagnetic

Answer: _____**False**_____

(d) For n = 1, the only allowed values for the angular momentum quantum numbers are ($\ell = 0, \mathrm{m} = 0$).

Answer: _____**True**_____

(e) A wave function $\psi_{n\ell m}(r, \theta, \phi)$ for a one-electron atom in the state $(\mathrm{n}, \ell, \mathrm{m})$ is called an orbital.

Answer: _____**True**_____

2. (Total 8 pts) **For each of the following pairs of atoms or ions, which one do you expect to have the larger radius? (+1 pt each) Briefly explain your answer as well. (+1 pt each)**

+1 pt each for the correct answer.
+1 pt each for the correct explanation.

(a) (2 pts) **N^{3-} or N**
Answer: ____**N^{3-}**_____

N^{3-} with extra electrons in 2p orbitals is larger than N due to **electron-electron repulsions**.

(b) (2 pts) **Ar or Ca**
Answer: ____**Ca**_____

Ca is larger than Ar since the **extra outer electrons beyond the Ar closed shell** are present.

(c) (2 pts) **Y or Cd**
Answer: ____**Y**_____

Y is larger than Cd since the **effective nuclear charge** increases through the transition series from Y to Cd.

(d) (2 pts) **Sr^{+} or Rb**
Answer: ____**Rb**_____

Sr^{+} and Rb have the same number of electrons, however, the **nuclear charge** of Sr^{+} is larger than Rb.

3. (Total 13 pts) The beryllium atom with Z = 4 has electron configuration Be: $(1s)^2(2s)^2$.
Answer the questions below **using the following table for the effective nuclear charges of atoms**.

(a) (**1 pts**) **Write the atomic wave function for a Be atom.**

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \mathbf{r}_4) = [\varphi_{1s}(r_1)\varphi_{1s}(r_2)][\varphi_{2s}(r_3)\varphi_{2s}(r_4)]$$

(b) (4 pts) **Calculate all possible first ionization energies for a Be atom in the unit of Ry. Use the Koopmans's approximation,** $IE_\alpha = -\epsilon_\alpha$.
+2 pt each for the correct answer. ***No partial points for wrong answers.***

$\mathrm{IE}_\alpha = -\epsilon_\alpha$; Koopmans's approximation

$\epsilon_n = -\frac{[Z_{eff}(n)]^2}{n^2}\ (Ry)$ …… the equation [5.9] in the textbook.

$\mathrm{IE}_{1s} = -\epsilon_{1s} = \frac{(3.68)^2}{1^2} = \mathbf{13.54\ Ry}$ …… **+2 pt**

$\mathrm{IE}_{2s} = -\epsilon_{2s} = \frac{(1.91)^2}{2^2} = \mathbf{0.91\ Ry}$ …… **+2 pt**

(c) (4 pts) **Calculate the kinetic energies in the unit of Ry when the atom is irradiated by X-ray with 50 Ry. Assume that the second ionization energies are much larger than the radiation energy.**
+2 pt each for the correct answer. ***No partial points for the wrong answers*****.**

$\mathbf{IE = E_{photon} - KE_{electron}}$ …… the equation [5.11] in the textbook.

$\mathrm{KE}_{\mathrm{electron}} = \mathrm{E}_{\mathrm{photon}} - IE$

Use the IE values of each orbital from 3(c).

$\mathrm{KE}_{1s} = 50\ \mathrm{Ry} - 13.54\ \mathrm{Ry} = \mathbf{36.46\ Ry}$ …… **+2 pt**

$\mathrm{KE}_{2s} = 50\ \mathrm{Ry} - 0.91\ \mathrm{Ry} = \mathbf{49.09\ Ry}$ …… **+2 pt**

(d) (4 pts) **Estimate the radius of the 1s and 2s orbitals using the equation below.**

$$\bar{r}_{nl} = \frac{(n)^2 a_0}{Z_{eff}(n)}\left\{1 + \frac{1}{2}\left[1 - \frac{l(l+1)}{n^2}\right]\right\}$$

+2 pt each for the correct answer. ***No partial points for the wrong answers*****.**
0.22 Å and **1.66** Å are also correct answers (a_0 = 5.291 10^{-11} m).

$\bar{r}_{1s} = -\frac{1^2 a_0}{3.68}\left\{1 + \frac{1}{2}\left[1 - \frac{0(0+1)}{1^2}\right]\right\} = \frac{a_0}{3.68} * \frac{3}{2} = \mathbf{0.41 a_0}$ …… **+2 pt**

$\bar{r}_{2s} = -\frac{2^2 a_0}{1.91}\left\{1 + \frac{1}{2}\left[1 - \frac{0(0+1)}{1^2}\right]\right\} = \frac{4a_0}{1.91} * \frac{3}{2} = \mathbf{3.14 a_0}$ …… **+2 pt**

4. (Total 9 pts) Answer the following questions.

(a) (2 pts) **Give <u>all values of quantum numbers (ℓ, m)</u> with n = 2 for one-electron atoms. You need to give the <u>name of the orbitals</u> as well.**

+2 pt for the correct answer

*** All quantum number sets (# = 4) should be written. *If not*, 1 pt will be deducted.**

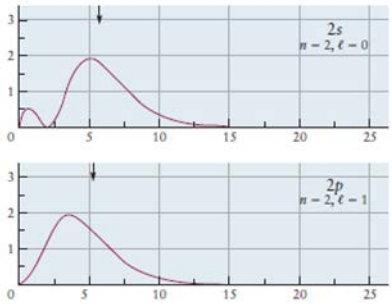
*** The quantum number and the name of orbitals should be matched. *If not*, 1 pt will be deducted.**

(0, 0): "<u>2s</u>" **…… +1 pt**

(1, -1), (1, 0), (1, 1): "<u>$2p_x$, $2p_y$, $2p_z$</u>" or "<u>2p</u>" **…… +1 pt**

(b) (3 pts) **Plot radial probability densities $r^2[R_{n\ell}(r)]^2$ on distance from the nucleus for each one-electron orbital.**

+1.5 pt each for the correct answer (*right pairs* of each orbital and its plot).



(c) (4 pts) **Compare the energy-level diagrams for all orbitals for a one-electron atom to a many-electron atom. Explain your answer.**

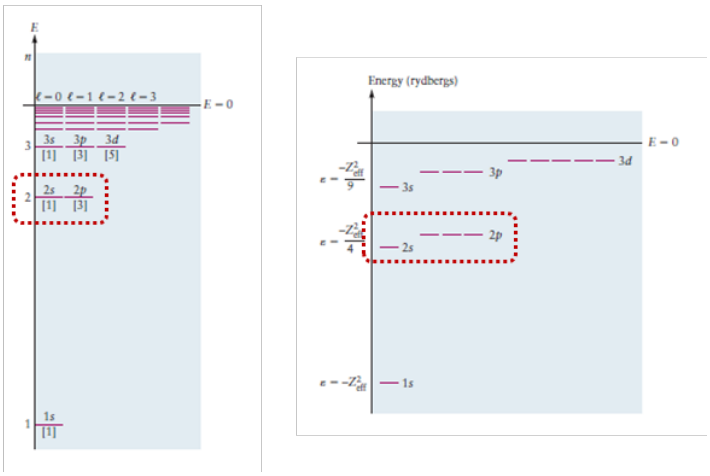
Plot of the energy-level diagrams (total 2 pts); Please see the red boxes below.

* 0.5 pt each will be deducted for the wrong number of orbitals.

Explanation (total 2 pts):

+1 pt each for a proper explanation regarding the quantum numbers

One-electron atom **Many-electron atom**



- One-electron atom: **n** contributes to the energy level. **… 1 pt**
- Many-electron atom: Both **n** and ℓ contribute to the energy level due to the **shielding effects** of different subshells; $\varepsilon_{ns} < \varepsilon_{np} < \varepsilon_{nd}$. **… 1 pt**