2. (**Kasap 1.1) Virial Theorem**

a) The Li atom has a nucleus with a *+3e* charge, which is surrounded by a full *1s* shell with two electrons, and a single valence electron in the outer *2s* subshell. The atomic radius of the Li atom is about 0.17 nm. Using the Virial theorem, and assuming the valence electron sees the nuclear *+3e* shielded by the two *1s* electrons, that is, a net charge of *+e*, estimate the ionization energy of Li (the energy required to free the *2s* electron). Compare this value with the experimental value of 5.39 eV.

b) Suppose the actual nuclear charge seen by the valence electron is not *+e* but a little higher, say *+1.25e*, due to the imperfect shielding provided by the closed *1s* shell. What would be the new ionization energy? What is your conclusion?

$r = 0.17\text{nm}$

$q_{net} = +e$

$e = 1.602\times10^{-19}\text{C}$

$k = 9.0\times10^{9}\ \text{Nm}^2/\text{C}^2$

$$PE = -\frac{k q_{net} e}{r} = -\frac{ke^2}{r} = -\frac{(9\times10^9\ \text{Nm}^2/\text{C}^2)(1.602\times10^{-19}\text{C})^2}{0.17\times10^{-9}\text{m}} =$$

$$= -1.359\times10^{-18}\text{J} \times \frac{1\text{eV}}{1.602\times10^{-19}\text{J}} = -8.48\text{ eV}$$

Virial theorem:

$$\overline{E} = \overline{KE} + \overline{PE} \quad \text{and} \quad \overline{KE} = -\frac{1}{2}\overline{PE}$$

then

$$\overline{E} = -\frac{1}{2}\overline{PE} + \overline{PE} = \frac{1}{2}\overline{PE} = -\frac{8.48\text{eV}}{2} = -4.24\text{ eV}$$

if $q_{net} = +1.25e$, then

$$PE = -1.25\frac{ke^2}{r} = -10.6\text{ eV}$$

$$\overline{E} = \frac{1}{2}\overline{PE} = -5.3\text{ eV}$$

This is closer to the experimental value, so the second assumption seems more realistic.

1. A) Summarize Bohr's model of the atom:

B) Allowed values for the quantum numbers of electrons are as follows:

$n = 1, 2, 3, \ldots$	(shell)
$l = 0, 1, 2, 3, \ldots, n - 1$	(subshell)
$m_l = 0, \pm 1, \pm 2, \ldots, \pm l$	(energy levels within a subshell)
$m_s = \pm \frac{1}{2}$	(spin – Pauli exclusion principle)

For the K shell, the four quantum numbers for each of the two electrons in the 1s state in the order of nlm_lm_s are 100(½) and 100(-½). Write the four quantum numbers for all of the electrons in the L and M shells, and note which correspond to the s, p, and d subshells.

C) Give the electron configurations for the following ions: P^{5+}, Se^{2-}, Ni^{2+}.

D) With regard to electron configuration, what do all the elements in group IIA of the periodic table have in common?

A) Electrons revolve around the atomic nucleus in circular orbits. The energies of the electrons are quantized, that is, electrons can only have certain allowed energy values. This leads to discrete orbits, i.e. only orbits of certain radii are allowed. An electron may change energy, but it must go to an allowed higher energy (with absorption of energy) or to a lower energy level (with emission of energy).

B) L state:

$n = 2$

$l = 0, 1$

$m_l = 0, \pm 1$

$m_s = \pm \frac{1}{2}$

200(½), 200(-½) } s subshell

210 (½), 210 (-½), 211 (½), 211 (-½), 21-1 (½), 21-1 (-½) } p subshell

M state:

$n = 3$

$\ell = 0, 1, 2$

$m_\ell = 0, \pm 1, \pm 2$

$m_s = \pm 1/2$

300(1/2)
300(-1/2) } s subshell

310(1/2)
310(-1/2)
311(1/2)
311(-1/2)
31-1(1/2)
31-1(-1/2) } p subshell

320(1/2)
320(-1/2)
321(1/2)
321(-1/2)
32-1(1/2)
32-1(-1/2)
322(1/2)
322(-1/2)
32-2(1/2)
32(-2)(-1/2) } d subshell

c) The neutral atoms are: ^{15}P, ^{34}Se, ^{28}Ni, then

P^{5+}: $1s^2 2s^2 2p^6$

Se^{2-}: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

Ni^{2+}: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8$

D) Each of the elements has two s- electrons.