Inorganic 09348 2001

Quiz I

September 21, 2001

Question 1 - Use the Rydberg Equation in order to calculate the ionization of one mole of H atoms.

$$\frac{1}{\lambda} = R\times\left(\frac{1}{{n_1}^2}-\frac{1}{{n_2}^2}\right) \text{ The energy of a photon is } \Delta E = \frac{c}{\lambda}h \Rightarrow \Delta E = chR\times\left(\frac{1}{{n_1}^2}-\frac{1}{{n_2}^2}\right)$$

When H is ionized the electron in $n_1 = 1$ goes to $n_2 = \infty$. So, the ionization energy is

$$IE = chR\times\left(\frac{1}{1^2}\right) \Rightarrow IE = 3\times10^{8}\times6.626\times10^{-34}\times1.097\times10^{7} = 2.1806\times10^{-18}\text{ J per atom}$$

or $IE = 2.1806\times10^{-18}\times6.02\times10^{23} = 1313\,\text{kJ.mol}^{-1} \Leftrightarrow \boxed{IE = 1313\,\text{kJ.mol}^{-1}}$

Question 2 - Use the Slater Rules in order to estimate IE(1) and EA(1) for Al.

$$E = -1312\times\frac{1}{n^2}\times\left(Z^*\right)^2 \quad \left[\text{kJ.mol}^{-1}\right]$$

Al (Z=13)

$\text{Al}\rightarrow 1s^2 2s^2 2p^6 3s^2 3p^1$ in Slater groups $\text{Al}\rightarrow(1s^2)(2s^2 2p^6)(3s^2 3p^1)$

$\text{Al}^+ \rightarrow 1s^2 2s^2 2p^6 3s^2$ in Slater groups $\text{Al}^+ \rightarrow (1s^2)(2s^2 2p^6)(3s^2 3p^o)$

$\text{Al}^- \rightarrow 1s^2 2s^2 2p^6 3s^2 3p^2$ in Slater groups $\text{Al}^- \rightarrow (1s^2)(2s^2 2p^6)(3s^2 3p^2)$

$Z^*\left(\text{Al, any } e^- \text{ from } 3s3p \text{ Slater group}\right) = 13-(2\times0.35+8\times0.85+2\times1) \Leftrightarrow$

$\Leftrightarrow \boxed{Z^*\left(\text{Al, any } e^- \text{ from } 3s3p \text{ Slater group}\right) = 3.5}$

$Z^*\left(\text{Al}^+\text{, any } e^- \text{ from } 3s3p \text{ Slater group}\right) = 13-(1\times0.35+8\times0.85+2\times1) \Leftrightarrow$

$\Leftrightarrow \boxed{Z^*\left(\text{Al}^+\text{, any } e^- \text{ from } 3s3p \text{ Slater group}\right) = 3.85}$

$Z^*\left(\text{Al}^-\text{, any } e^- \text{ from } 3s3p \text{ Slater group}\right) = 13-(3\times0.35+8\times0.85+2\times1) \Leftrightarrow$

$\Leftrightarrow \boxed{Z^*\left(\text{Al}^-\text{, any } e^- \text{ from } 3s3p \text{ Slater group}\right) = 3.15}$

As we need to calculate the difference in energy we don't have to calculate the energies of the electrons that don't change their energies, because these energies will cancel out. So, one only as to consider the electrons of the last Slater group.

IE: $\text{Al} \rightarrow \text{Al}^+ + e^-$

$$IE(\text{Al}) = E(\text{Al}^+) - E(\text{Al}) \quad \Rightarrow \quad IE(\text{Al}) = \left(-1312\times\frac{1}{9}\times(3.85)^2\times2\right)-\left(-1312\times\frac{1}{9}\times(3.5)^2\times3\right) \Leftrightarrow$$

$\Leftrightarrow \boxed{IE(\text{Al}) = 1036\,\text{kJ.mol}^{-1}}$

EA: $\text{Al} + e^- \rightarrow \text{Al}^-$

$$EA(\text{Al}) = E(\text{Al}^-) - E(\text{Al}) \quad \Rightarrow \quad EA(\text{Al}) = \left(-1312\times\frac{1}{9}\times(3.15)^2\times4\right)-\left(-1312\times\frac{1}{9}\times(3.5)^2\times3\right) \Leftrightarrow$$

$\Leftrightarrow \boxed{EA(\text{Al}) = -429\,\text{kJ.mol}^{-1}}$

Question 3 - Show how DeBroglie used Einstein's equation to justify his newly found relationship:

$$\lambda = \frac{h}{p}$$

Einstein's energy mass equivalency is

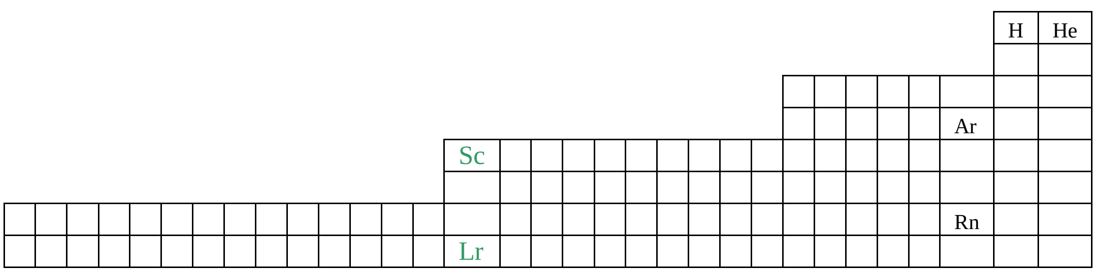
$$E = m.c^2 \Leftrightarrow E = mcc \Rightarrow E = pc$$

But for a photon $c = \lambda \nu$ and $E = h\nu \Rightarrow h\nu = p\lambda\nu \Leftrightarrow \boxed{\lambda = \frac{h}{p}}$

Question 4 - Write down the electronic configuration of Sc (*Z*=21) and Lr (*Z*=103). Place these elements in their correct positions en the "long' versions of the Periodic Table.

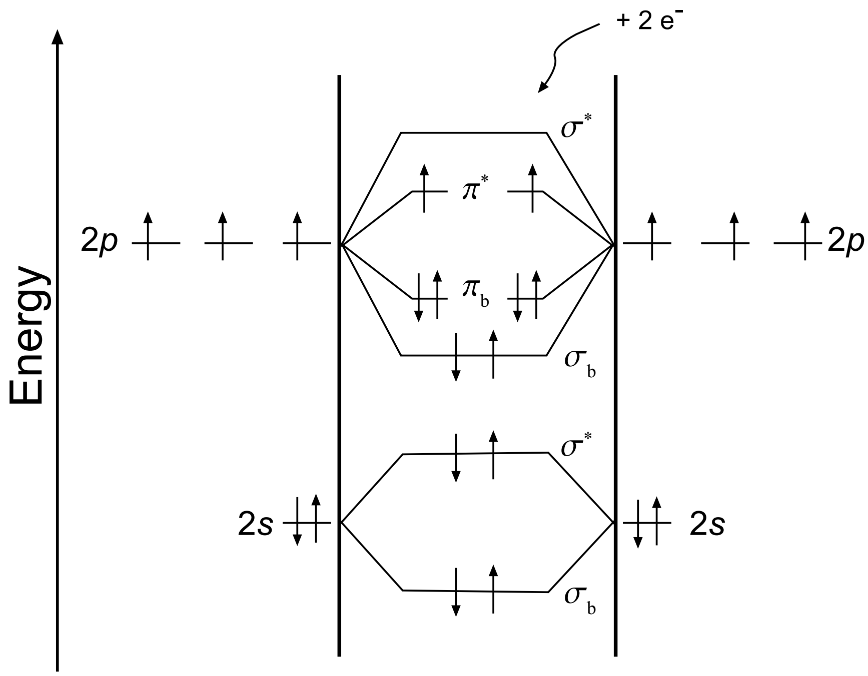
Sc (*Z*=21)
$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^1$

Lr (*Z*=103)
$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 5f^{14} 6d^1$



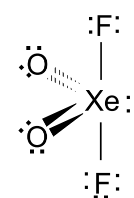
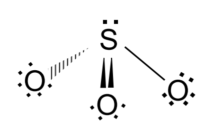
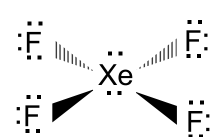
Question 5 - Complete the MO diagram for N_2^{2-}:

$N \rightarrow 1s^2 2s^2 2p^3$. So, N atom has 5 valence electrons. This means that the anion N_2^{2-} has 5+5+2=12 electrons that contribute to the bond(s).



There are eight bonding electrons: four from σ_b and four from π_b. There are 4 anti-bonding electrons: two from σ^* and two from π^*. So, the bonding order is $\frac{8-4}{2} = 2$.

Question 6 - Decide on the number of electron domains found around the central atom in each of the following molecules/ions.

Compound	Number of domains	Shape of the array of the domains	Sketch of the molecule/Ion
XeO_2F_2	5	Trigonal bipyramidal	
SO_3^{2-}	4	Tetrahedral	
XeF_4	6	Octahedral	
BeH_2	2	Linear	H — Be — H

Question 7 - Derive the Rydberg Equation from the combination of the Newton-Coulomb relation with the Bohr quantum postulate.

$$\begin{cases} \text{Coulomb force} = \text{Centrifugal force} \\ \\ \text{Bohr quantization of angular moment} \end{cases} \Rightarrow \begin{cases} \dfrac{1}{4\pi\varepsilon_o}\dfrac{Ze^2}{r^2} = m\dfrac{v^2}{r} \\ \\ mvr = n\dfrac{h}{2\pi} \end{cases} \Leftrightarrow \begin{cases} r = \dfrac{\varepsilon_o h^2}{Zm\pi e^2}n^2 \\ \\ v = \dfrac{Ze^2}{2\varepsilon_o h}\times\dfrac{1}{n} \end{cases}$$

The energy E of an electron is the sum of its potential energy, V, and is kinetic energy, E_k.

$$V = \int_{\infty}^{r}\frac{1}{4\pi\varepsilon_o}\frac{Ze^2}{r^2}dr \Leftrightarrow V = -\frac{1}{4\pi\varepsilon_o}\frac{Ze^2}{r} \qquad\qquad E_k = \frac{1}{2}mv^2 \Rightarrow E_k = \frac{Z^2e^4m}{8\varepsilon_o h^2}\times\frac{1}{n^2}$$

$$E = V + E_k \Rightarrow E = -\frac{Z^2e^4m}{8\varepsilon_o{}^2h^2}\times\frac{1}{n^2}$$

Suppose one have a transition from an n_2 level to an n_1 level, with $n_2 > n_1$. The difference in energies would be

$$\Delta E = E_2 - E_1 = \frac{Z^2e^4m}{8\varepsilon_o{}^2h^2}\times\left(\frac{1}{n_1{}^2} - \frac{1}{n_2{}^2}\right) \qquad\qquad \text{but } \Delta E = \frac{1}{\lambda}hc$$

so,

$$\frac{1}{\lambda} = \frac{Z^2e^4m}{8\varepsilon_o{}^2h^3c}\times\left(\frac{1}{n_1{}^2} - \frac{1}{n_2{}^2}\right)$$

or

$$\boxed{\frac{1}{\lambda} = R\times\left(\frac{1}{n_1{}^2} - \frac{1}{n_2{}^2}\right)} \text{ where } R = \frac{Z^2e^4m}{8\varepsilon_o{}^2h^3c} \text{ is the Rydberg constant.}$$