Homework 1

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1. (a) First and foremost, we want to calculate the percent by mass. We know that percent may be expressed as:

$$\% = \frac{\text{Contribution of Component}}{\text{Total Mass}}$$

Given that w represents the weight fraction of an element, and M represents the atomic mass of an element, we may express the contribution of a single i-th element as:

$$m_i = \frac{w_i}{M_i}$$

For an alloy consisting of N elements, we can find the total mass by summing the individual contribution of each element, up to N:

$$m_{tot} = \frac{w_1}{M_1} + \frac{w_2}{M_2} + \cdots + \frac{w_N}{M_N}$$

We then combine the two above expressions to get:

$$\boxed{n_i = \frac{\dfrac{w_i}{M_i}}{\dfrac{w_1}{M_1} + \dfrac{w_2}{M_2} + \cdots + \dfrac{w_N}{M_N}}}$$

(b) We can reverse the molar mass obtained in part (a) and re-express the weight fraction in terms of it. We follow a similar process to obtain the individual contribution:

$$w_i = n_i M_i$$

We then find the total as:

$$w_{tot} = n_A M_A + n_B M_B + \cdots + n_N M_N$$

Thus, we once again obtain a general expression:

$$w_i = \frac{n_i M_i}{n_A M_A + n_B M_B + \cdots + n_N M_N}$$

(c) Per the periodic table, we may obtain the atomic masses as:

$$n_{Cd} = 112.41 \left[\frac{g}{mol}\right]$$

$$n_{Se} = 78.96 \left[\frac{g}{mol}\right]$$

Given that there is only one of each atom, we may write:

$$\%_{Cd} = \frac{112.41}{112.41 + 78.96} = .5874$$

$$\%_{Se} = 1 - .5874 = .4126$$

Thus, per 100 grams of CdSe, we would find:

$$m_{Cd} = 58.74[g]$$

$$m_{Se} = 41.26[g]$$

(d) Using our equations from before, along with atomic masses obtained from the periodic table, we can find:

$$\%_{Se} = \frac{\frac{.77}{78.96}}{\frac{.77}{78.96} + \frac{.2}{127.6} + \frac{.03}{30.974}}$$

$$\%_{Se} = .7936$$

$$\%_{Te} = \frac{\frac{.2}{127.6}}{\frac{.77}{78.96} + \frac{.2}{127.6} + \frac{.03}{30.974}}$$

$$\%_{Te} = .1276$$

$$\%_P = 1 - .7936 - .1276$$

$$\%_P = .078842$$

2. (a) We may use Coulomb's law to identify the potential energies of all actors in the picture. Thus, we need to check the electron-electron interaction, proton-proton interaction, and the interaction of both electron-proton pairs. For this, we should note that electrons have a charge $-e$, while protons have a charge $+e$. Thus, let us denote the left-most electron as e_1, the right-most electron as e_2, and, similarly, the left-most proton as p_1 and the right-most proton as p_2. This yields:

$$PE_{e_1 p_1 p_2} = \frac{-e^2}{4\pi\varepsilon_o r_o} + \frac{-e^2}{4\pi\varepsilon_o(3r_o)}$$

$$PE_{e_2 p_1 p_2 e_1} = \frac{-e^2}{4\pi\varepsilon_o r_o} + \frac{-e^2}{4\pi\varepsilon_o r_o} + \frac{e^2}{4\pi\varepsilon_o(2r_o)}$$

$$PE_{p_1 p_2} = \frac{e^2}{4\pi\varepsilon_o(2r_o)}$$

By superposition we then sum each case to get:

$$PE_{tot} = \frac{e^2}{8\pi\varepsilon_o r_o} - \frac{3e^2}{8\pi\varepsilon_o r_o} - \frac{e^2}{3\pi\varepsilon_o r_o}$$

$$PE_{tot} = -\frac{7e^2}{12\pi\varepsilon_o r_o}$$

We can then substitute our known values to get:

$$PE_{tot} = -\frac{7\left(1.6\cdot 10^{-19}\right)^2}{12\pi\left(8.85\cdot 10^{-12}\right)\left(.0529\cdot 10^{-9}\right)}$$

$$\boxed{PE_{tot} = -1.0153\cdot 10^{-17}[\text{J}] = -63.377[\text{eV}]}$$

Thus, we may see that, because the total energy is negative, this arrangement is favorable.

(b) We may write the energy of an isolated hydrogen as:

$$E_{\text{H}} = 2(-13.6) = -27.2[\text{eV}]$$

We may see that the difference in the above arrangement and two isolated hydrogen atoms is:

$$\Delta PE = -63.377 - 2(-27.2) = -8.977[\text{eV}]$$

Using the Virial theorem, the change in covalent bond energy is then:

$$\Delta E = \frac{1}{2}\Delta PE$$

$$\boxed{\Delta E = -4.4885[\text{eV}]}$$

As such, we see that the overall energy of the shown arrangement yields a lower potential energy than two isolated hydrogen atoms; therefore, the arrangement is energetically favorable. We may observe that our calculated value differs by the experimental $-4.51[\langle\rangle]$ by $< .5\%$, and is therefore negligible.

3. First and foremost, we are given the energy as:

$$E(r) = -\frac{e^2 M}{4\pi\varepsilon_o r} + \frac{B}{r^m}$$

We must recall that, at an equilibrium, the energy is zero, and, therefore, we want:

$$0 = \frac{d}{dr}\left[-\frac{e^2 M}{4\pi\varepsilon_o r_o} + \frac{B}{r_o^m}\right]$$

We may rearrange to solve for the radius:

$$\frac{e^2 M}{4\pi\varepsilon_o r_o^2} = \frac{mB}{r_o^{m+1}}$$

$$r_o^{m-1} = \frac{36\pi\varepsilon_o B}{e^2 M}$$

Plugging in known values, we may solve to get:

$$r_o = \sqrt[8]{\frac{36\pi(8.85 \cdot 10^{-12})(1.192 \cdot 10^{-104})}{(1.6 \cdot 10^{-19})^2(1.763)}}$$

$$\boxed{r_o = 3.56 \cdot 10^{-10}[\text{m}] = 3.56[\text{Å}]}$$

We then substitute this into the formula for energy to get:

$$E(r_o) = -\frac{e^2 M}{4\pi\varepsilon_o r_o} + \frac{B}{r^m}$$

$$E(r_o) = -\frac{(1.6 \cdot 10^{-19})^2(1.763)}{4\pi(8.85 \cdot 10^{-12})(3.56 \cdot 10^{-10})} + \frac{1.192 \cdot 10^{-104}}{(3.56 \cdot 10^{-10})^9}$$

This gives us:

$$\boxed{E(r_o) = -1.0125 \cdot 10^{-18}[\text{J}] = -6.319528[\langle\rangle]}$$