EXAMPLE PROBLEM 2.1

Average Atomic Weight Computation for Cerium

Cerium has four naturally occurring isotopes: 0.185% of ^{136}Ce, with an atomic weight of 135.907 amu; 0.251% of ^{138}Ce, with an atomic weight of 137.906 amu; 88.450% of ^{140}Ce, with an atomic weight of 139.905 amu; and 11.114% of ^{142}Ce, with an atomic weight of 141.909 amu. Calculate the average atomic weight of Ce.

Solution

The average atomic weight of a hypothetical element M, $\overline{A}_{\mathrm{M}}$, is computed by adding fraction-of-occurrence—atomic weight products for all its isotopes; that is,

$$\overline{A}_{\mathrm{M}} = \sum_i f_{i_{\mathrm{M}}} A_{i_{\mathrm{M}}} \tag{2.2}$$

In this expression, $f_{i_{\mathrm{M}}}$ is the fraction-of-occurrence of isotope i for element M (i.e., the percentage-of-occurrence divided by 100), and $A_{i_{\mathrm{M}}}$ is the atomic weight of the isotope.

For cerium, Equation 2.2 takes the form

$$\overline{A}_{\mathrm{Ce}} = f_{^{136}\mathrm{Ce}} A_{^{136}\mathrm{Ce}} + f_{^{138}\mathrm{Ce}} A_{^{138}\mathrm{Ce}} + f_{^{140}\mathrm{Ce}} A_{^{140}\mathrm{Ce}} + f_{^{142}\mathrm{Ce}} A_{^{142}\mathrm{Ce}}$$

Incorporating values provided in the problem statement for the several parameters leads to

$$\begin{aligned}\overline{A}_{\mathrm{Ce}} &= \left(\frac{0.185\%}{100}\right)(135.907\text{ amu}) + \left(\frac{0.251\%}{100}\right)(137.906\text{ amu}) + \left(\frac{88.450\%}{100}\right)(139.905\text{ amu}) \\ &\quad + \left(\frac{11.114\%}{100}\right)(141.909\text{ amu}) \\ &= (0.00185)(135.907\text{ amu}) + (0.00251)(137.906\text{ amu}) + (0.8845)(139.905\text{ amu}) \\ &\quad + (0.11114)(141.909\text{ amu}) \\ &= 140.115\text{ amu}\end{aligned}$$

EXAMPLE PROBLEM 2.2

Computation of Attractive and Repulsive Forces between Two Ions

The atomic radii of K^+ and Br^- ions are 0.138 and 0.196 nm, respectively.

(a) Using Equations 2.9 and 2.10, calculate the force of attraction between these two ions at their equilibrium interionic separation (i.e., when the ions just touch one another).
(b) What is the force of repulsion at this same separation distance?

Solution

(a) From Equation 2.5b, the force of attraction between two ions is

$$F_A = \frac{dE_A}{dr}$$

Whereas, according to Equation 2.9,

$$E_A = -\frac{A}{r}$$

Now, taking the derivation of E_A with respect to r yields the following expression for the force of attraction F_A:

$$F_A = \frac{dE_A}{dr} = \frac{d\left(-\frac{A}{r}\right)}{dr} = -\left(\frac{-A}{r^2}\right) = \frac{A}{r^2} \tag{2.12}$$

Now substitution into this equation the expression for A (Eq. 2.10) gives

$$F_A = \frac{1}{4\pi\epsilon_0 r^2}(|Z_1|e)(|Z_2|e) \tag{2.13}$$

Incorporation into this equation values for e and ϵ_0 leads to

$$\begin{aligned} F_A &= \frac{1}{4\pi(8.85 \times 10^{-12}\ \text{F/m})(r^2)}\left[|Z_1|(1.602 \times 10^{-19}\text{C})\right]\left[|Z_2|(1.602 \times 10^{-19}\text{C})\right] \\ &= \frac{(2.31 \times 10^{-28}\ \text{N}\cdot\text{m}^2)(|Z_1|)(|Z_2|)}{r^2} \end{aligned} \tag{2.14}$$

For this problem, r is taken as the interionic separation r_0 for KBr, which is equal to the sum of the K^+ and Br^- ionic radii inasmuch as the ions touch one another—that is,

$$\begin{aligned} r_0 &= r_{K^+} + r_{Br^-} \\ &= 0.138\ \text{nm} + 0.196\ \text{nm} \\ &= 0.334\ \text{nm} \\ &= 0.334 \times 10^{-9}\ \text{m} \end{aligned} \tag{2.15}$$

When we substitute this value for r into Equation 2.14, and taking ion 1 to be K^+ and ion 2 as Br^- (i.e., $Z_1 = +1$ and $Z_2 = -1$), then the force of attraction is equal to

$$F_A = \frac{(2.31 \times 10^{-28}\ \text{N}\cdot\text{m}^2)(|+1|)(|-1|)}{(0.334 \times 10^{-9}\ \text{m})^2} = 2.07 \times 10^{-9}\ \text{N}$$

(b) At the equilibrium separation distance the sum of attractive and repulsive forces is zero according to Equation 2.4. This means that

$$F_R = -F_A = -(2.07 \times 10^{-9}\ \text{N}) = -2.07 \times 10^{-9}\ \text{N}$$

EXAMPLE PROBLEM 2.3

Calculation of the Percent Ionic Character for the C-H Bond

Compute the percent ionic character (%IC) of the interatomic bond that forms between carbon and hydrogen.

Solution

The %IC of a bond between two atoms/ions, A and B (A being the more electronegative) is a function of their electronegativities X_A and X_B, according to Equation 2.16. The electronegativities for C and H (see Figure 2.9) are $X_C = 2.5$ and $X_H = 2.1$. Therefore, the %IC is

$$\begin{aligned}\%\text{IC} &= \{1 - \exp[-(0.25)(X_C - X_H)^2]\} \times 100 \\ &= \{1 - \exp[-(0.25)(2.5 - 2.1)^2]\} \times 100 \\ &= 3.9\%\end{aligned}$$

Thus the C—H atomic bond is primarily covalent (96.1%).

2.4 *Indium has two naturally occurring isotopes: ^{113}In with an atomic weight of 112.904 amu, and ^{115}In with an atomic weight of 114.904 amu. If the average atomic weight for In is 114.818 amu, calculate the fraction-of-occurrences of these two isotopes.*

Solution

The average atomic weight of indium $(\bar{A}_{In})$ is computed by adding fraction-of-occurrence—atomic weight products for the two isotopes—i.e., using Equation 2.2, or

$$\bar{A}_{In} = f_{^{113}In} A_{^{113}In} + f_{^{115}In} A_{^{115}In}$$

Because there are just two isotopes, the sum of the fracture-of-occurrences will be 1.000; or

$$f_{^{113}In} + f_{^{115}In} = 1.000$$

which means that

$$f_{^{113}In} = 1.000 - f_{^{115}In}$$

Substituting into this expression the one noted above for $f_{^{113}In}$, and incorporating the atomic weight values provided in the problem statement yields

$$114.818 \text{ amu} = f_{^{113}In} A_{^{113}In} + f_{^{115}In} A_{^{115}In}$$

$$114.818 \text{ amu} = (1.000 - f_{^{113}In}) A_{^{113}In} + f_{^{115}In} A_{^{115}In}$$

$$114.818 \text{ amu} = (1.000 - f_{^{115}In})(112.904 \text{ amu}) + f_{^{115}In}(114.904 \text{ amu})$$

$$114.818 \text{ amu} = 112.904 \text{ amu} - f_{^{115}In}(112.904 \text{ amu}) + f_{^{115}In}(114.904 \text{ amu})$$

Solving this expression for $f_{^{115}In}$ yields $f_{^{115}In} = 0.957$. Furthermore, because

$$f_{^{113}In} = 1.000 - f_{^{115}In}$$

then

$$f_{^{113}In} = 1.000 - 0.957 = 0.043$$

2.5 *(a) How many grams are there in one amu of a material?*

(b) Mole, in the context of this book, is taken in units of gram-mole. On this basis, how many atoms are there in a pound-mole of a substance?

Solution

(a) In order to determine the number of grams in one amu of material, appropriate manipulation of the amu/atom, g/mol, and atom/mol relationships is all that is necessary, as

$$\#\text{g/amu} = \left(\frac{1\,\text{mol}}{6.022\ \times\ 10^{23}\,\text{atoms}}\right)\left(\frac{1\,\text{g/mol}}{1\,\text{amu/atom}}\right)$$

$$= 1.66 \times 10^{-24}\ \text{g/amu}$$

(b) Since there are 453.6 g/lb$_m$,

$$1\ \text{lb-mol} = (453.6\ \text{g/lb}_m)(6.022\ \times\ 10^{23}\ \text{atoms/g-mol})$$

$$= 2.73 \times 10^{26}\ \text{atoms/lb-mol}$$

2.9 *Give the electron configurations for the following ions:* P^{5+}, P^{3-}, Sn^{4+}, Se^{2-}, I^{-}, *and* Ni^{2+}.

Solution

The electron configurations for the ions are determined using Table 2.2 (and Figure 2.8).

P^{5+}: From Table 2.2, the electron configuration for an atom of phosphorus is $1s^22s^22p^63s^23p^3$. In order to become an ion with a plus five charge, it must lose five electrons—in this case the three 3*p* and the two 3*s*. Thus, the electron configuration for a P^{5+} ion is $1s^22s^22p^6$.

P^{3-}: From Table 2.2, the electron configuration for an atom of phosphorus is $1s^22s^22p^63s^23p^3$. In order to become an ion with a minus three charge, it must acquire three electrons—in this case another three 3*p*. Thus, the electron configuration for a P^{3-} ion is $1s^22s^22p^63s^23p^6$.

Sn^{4+}: From the periodic table, Figure 2.8, the atomic number for tin is 50, which means that it has fifty electrons and an electron configuration of $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^2$. In order to become an ion with a plus four charge, it must lose four electrons—in this case the two 4*s* and two 5*p*. Thus, the electron configuration for an Sn^{4+} ion is $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}$.

Se^{2-}: From Table 2.2, the electron configuration for an atom of selenium is $1s^22s^22p^63s^23p^63d^{10}4s^24p^4$. In order to become an ion with a minus two charge, it must acquire two electrons—in this case another two 4*p*. Thus, the electron configuration for an Se^{2-} ion is $1s^22s^22p^63s^23p^63d^{10}4s^24p^6$.

I^{-}: From the periodic table, Figure 2.8, the atomic number for iodine is 53, which means that it has fifty three electrons and an electron configuration of $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^5$. In order to become an ion with a minus one charge, it must acquire one electron—in this case another 5*p*. Thus, the electron configuration for an I^{-} ion is $1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^6$.

Ni^{2+}: From Table 2.2, the electron configuration for an atom of nickel is $1s^22s^22p^63s^23p^63d^84s^2$. In order to become an ion with a plus two charge, it must lose two electrons—in this case the two 4*s*. Thus, the electron configuration for a Ni^{2+} ion is $1s^22s^22p^63s^23p^63d^8$.

2.13 *Without consulting Figure 2.8 or Table 2.2, determine whether each of the following electron configurations is an inert gas, a halogen, an alkali metal, an alkaline earth metal, or a transition metal. Justify your choices.*

(a) $1s^2 2s^2 2p^6 3s^2 3p^5$

(b) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$

(c) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$

(d) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

(e) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^5 5s^2$

(f) $1s^2 2s^2 2p^6 3s^2$

Solution

(a) The $1s^2 2s^2 2p^6 3s^2 3p^5$ electron configuration is that of a halogen because it is one electron deficient from having a filled *p* subshell.

(b) The $1s^2 2s^2 2p^6 3s^2 3p^6 3d^7 4s^2$ electron configuration is that of a transition metal because of an incomplete *d* subshell.

(c) The $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ electron configuration is that of an inert gas because of filled 4*s* and 4*p* subshells.

(d) The $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$ electron configuration is that of an alkali metal because of a single *s* electron.

(e) The $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^5 5s^2$ electron configuration is that of a transition metal because of an incomplete *d* subshell.

(f) The $1s^2 2s^2 2p^6 3s^2$ electron configuration is that of an alkaline earth metal because of two *s* electrons.

2.18 *The net potential energy between two adjacent ions,* E_N*, may be represented by the sum of Equations 2.9 and 2.11; that is,*

$$E_N = -\frac{A}{r} + \frac{B}{r^n} \qquad (2.17)$$

Calculate the bonding energy E_0 *in terms of the parameters A, B, and n using the following procedure:*

1. Differentiate E_N *with respect to r, and then set the resulting expression equal to zero, since the curve of* E_N *versus r is a minimum at* E_0*.*

2. Solve for r in terms of A, B, and n, which yields r_0*, the equilibrium interionic spacing.*

3. Determine the expression for E_0 *by substitution of* r_0 *into Equation 2.17.*

<u>Solution</u>

(a) Differentiation of Equation 2.17 yields

$$\frac{dE_N}{dr} = \frac{d\left(-\frac{A}{r}\right)}{dr} + \frac{d\left(\frac{B}{r^n}\right)}{dr}$$

$$= \frac{A}{r^{(1+1)}} - \frac{nB}{r^{(n+1)}} = 0$$

(b) Now, solving for r (= r_0)

$$\frac{A}{r_0^2} = \frac{nB}{r_0^{(n+1)}}$$

or

$$r_0 = \left(\frac{A}{nB}\right)^{1/(1-n)}$$

(c) Substitution for r_0 into Equation 2.17 and solving for E (= E_0) yields

$$E_0 = -\frac{A}{r_0} + \frac{B}{r_0^n}$$

$$= -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1-n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1-n)}}$$

Fundamentals of Engineering Questions and Problems

2.1FE *The chemical composition of the repeat unit for nylon 6,6 is given by the formula* $C_{12}H_{22}N_2O_2$. *Atomic weights for the constituent elements are* $A_C = 12$, $A_H = 1$, $A_N = 14$, *and* $A_O = 16$. *According to this chemical formula (for nylon 6,6), the percent (by weight) of carbon in nylon 6,6 is most nearly:*

(A) 31.6%

(B) 4.3%

(C) 14.2%

(D) 63.7%

Solution

The total atomic weight of one repeat unit of nylon 6,6, A_{total}, is calculated as

$$A_{total} = (12 \text{ atoms})(A_C) + (22 \text{ atoms})(A_H) + (2 \text{ atoms})(A_N) + (2 \text{ atoms})(A_O)$$

$$= (12 \text{ atoms})(12 \text{ g/mol}) + (22 \text{ atoms})(1 \text{ g/mol}) + (2 \text{ atoms})(14 \text{ g/mol}) + (2 \text{ atoms})(16 \text{ g/mol}) = 226 \text{ g/mol}$$

Therefore the percent by weight of carbon is calculated as

$$\text{C(wt\%)} = \frac{(12 \text{ atoms})(A_C)}{A_{\text{total}}} \times 100$$

$$= \frac{(12 \text{ atoms})(12 \text{ g/mol})}{226 \text{ g/mol}} \times 100 = 63.7\%$$

which is answer D.