

## EXAMPLE PROBLEM 2.1

### Average Atomic Weight Computation for Cerium

Cerium has four naturally occurring isotopes: 0.185% of  $^{136}\text{Ce}$ , with an atomic weight of 135.907 amu; 0.251% of  $^{138}\text{Ce}$ , with an atomic weight of 137.906 amu; 88.450% of  $^{140}\text{Ce}$ , with an atomic weight of 139.905 amu; and 11.114% of  $^{142}\text{Ce}$ , 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,  $\bar{A}_M$ , is computed by adding fraction-of-occurrence—atomic weight products for all its isotopes; that is,

$$\bar{A}_M = \sum_i f_{iM} A_{iM} \quad (2.2)$$

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

For cerium, Equation 2.2 takes the form

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

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

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

## EXAMPLE PROBLEM 2.2

### Computation of Attractive and Repulsive Forces between Two Ions

The atomic radii of  $\text{K}^+$  and  $\text{Br}^-$  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  $F_A$ :

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

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

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

Incorporation into this equation values for  $e$  and  $\epsilon_0$  leads to

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

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

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

When we substitute this value for  $r$  into Equation 2.14, and taking ion 1 to be  $\text{K}^+$  and ion 2 as  $\text{Br}^-$  (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

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

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

2.4 Indium has two naturally occurring isotopes:  $^{113}\text{In}$  with an atomic weight of 112.904 amu, and  $^{115}\text{In}$  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 ( $\bar{A}_{\text{In}}$ ) is computed by adding fraction-of-occurrence—atomic weight products for the two isotopes—i.e., using Equation 2.2, or

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

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

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

which means that

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

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

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

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

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

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

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

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

then

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

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

$$\begin{aligned}\#g/\text{amu} &= \left( \frac{1 \text{ mol}}{6.022 \times 10^{23} \text{ atoms}} \right) \left( \frac{1 \text{ g/mol}}{1 \text{ amu/atom}} \right) \\ &= 1.66 \times 10^{-24} \text{ g/amu}\end{aligned}$$

(b) Since there are 453.6 g/lb<sub>m</sub>,

$$\begin{aligned}1 \text{ lb-mol} &= (453.6 \text{ g/lb}_m)(6.022 \times 10^{23} \text{ atoms/g-mol}) \\ &= 2.73 \times 10^{26} \text{ atoms/lb-mol}\end{aligned}$$

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  $1s^2 2s^2 2p^6 3s^2 3p^3$ . In order to become an ion with a plus five charge, it must lose five electrons—in this case the three  $3p$  and the two  $3s$ . Thus, the electron configuration for a  $P^{5+}$  ion is  $1s^2 2s^2 2p^6$ .

$P^{3-}$ : From Table 2.2, the electron configuration for an atom of phosphorus is  $1s^2 2s^2 2p^6 3s^2 3p^3$ . In order to become an ion with a minus three charge, it must acquire three electrons—in this case another three  $3p$ . Thus, the electron configuration for a  $P^{3-}$  ion is  $1s^2 2s^2 2p^6 3s^2 3p^6$ .

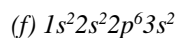
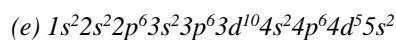
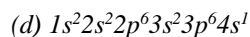
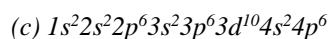
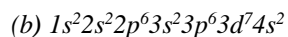
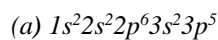
$Sn^{4+}$ : From the periodic table, Figure 2.8, the atomic number for tin is 50, which means that it has fifty electrons and an electron configuration of  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^2$ . In order to become an ion with a plus four charge, it must lose four electrons—in this case the two  $4s$  and two  $5p$ . Thus, the electron configuration for an  $Sn^{4+}$  ion is  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10}$ .

$Se^{2-}$ : From Table 2.2, the electron configuration for an atom of selenium is  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^4$ . In order to become an ion with a minus two charge, it must acquire two electrons—in this case another two  $4p$ . Thus, the electron configuration for an  $Se^{2-}$  ion is  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$ .

$I^-$ : 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  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^5$ . In order to become an ion with a minus one charge, it must acquire one electron—in this case another  $5p$ . Thus, the electron configuration for an  $I^-$  ion is  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6$ .

$Ni^{2+}$ : From Table 2.2, the electron configuration for an atom of nickel is  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$ . In order to become an ion with a plus two charge, it must lose two electrons—in this case the two  $4s$ . Thus, the electron configuration for a  $Ni^{2+}$  ion is  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8$ .

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.



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  $4s$  and  $4p$  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,

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

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.

### Solution

(a) Differentiation of Equation 2.17 yields

$$\begin{aligned} \frac{dE_N}{dr} &= \frac{d\left(-\frac{A}{r}\right)}{dr} + \frac{d\left(\frac{B}{r^n}\right)}{dr} \\ &= \frac{A}{r^{(1+1)}} - \frac{nB}{r^{(n+1)}} = 0 \end{aligned}$$

(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

$$\begin{aligned} E_0 &= -\frac{A}{r_0} + \frac{B}{r_0^n} \\ &= -\frac{A}{\left(\frac{A}{nB}\right)^{1/(1-n)}} + \frac{B}{\left(\frac{A}{nB}\right)^{n/(1-n)}} \end{aligned}$$

## 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

$$\begin{aligned} A_{total} &= (12 \text{ atoms})(A_C) + (22 \text{ atoms})(A_H) + (2 \text{ atoms})(A_N) + (2 \text{ atoms})(A_O) \\ &= (12 \text{ atoms})(12 \text{ g/mol}) + (22 \text{ atoms})(1 \text{ g/mol}) + (2 \text{ atoms})(14 \text{ g/mol}) + (2 \text{ atoms})(16 \text{ g/mol}) = 226 \text{ g/mol} \end{aligned}$$

Therefore the percent by weight of carbon is calculated as

$$\begin{aligned} C(\text{wt}\%) &= \frac{(12 \text{ atoms})(A_C)}{A_{total}} \cdot 100 \\ &= \frac{(12 \text{ atoms})(12 \text{ g/mol})}{226 \text{ g/mol}} \cdot 100 = 63.7\% \end{aligned}$$

which is answer D.