CHAPTER 2

ATOMIC STRUCTURE AND INTERATOMIC BONDING

PROBLEM SOLUTIONS

Fundamental Concepts

Electrons in Atoms

2.1 *Cite the difference between atomic mass and atomic weight.*

Solution

Atomic mass is the mass of an individual atom, whereas atomic weight is the average (weighted) of the atomic masses of an atom's naturally occurring isotopes.

2.2 *Silicon has three naturally occurring isotopes: 92.23% of* ^{28}*Si, with an atomic weight of 27.9769 amu, 4.68% of* ^{29}*Si, with an atomic weight of 28.9765 amu, and 3.09% of* ^{30}*Si, with an atomic weight of 29.9738 amu. On the basis of these data, confirm that the average atomic weight of Si is 28.0854 amu.*

Solution

The average atomic weight of silicon $(\bar{A}_{\text{Si}})$ is computed by adding fraction-of-occurrence/atomic weight products for the three isotopes—i.e., using Equation 2.2. (Remember: fraction of occurrence is equal to the percent of occurrence divided by 100.) Thus

$$\bar{A}_{\text{Si}} = f_{^{28}\text{Si}} A_{^{28}\text{Si}} + f_{^{29}\text{Si}} A_{^{29}\text{Si}} + f_{^{30}\text{Si}} A_{^{30}\text{Si}}$$

$$= (0.9223)(27.9769) + (0.0468)(28.9765) + (0.0309)(29.9738) = 28.0854$$

2.3 *Zinc has five naturally occurring isotopes: 48.63% of* ^{64}*Zn with an atomic weight of 63.929 amu; 27.90% of* ^{66}*Zn with an atomic weight of 65.926 amu; 4.10% of* ^{67}*Zn with an atomic weight of 66.927 amu; 18.75% of* ^{68}*Zn with an atomic weight of 67.925 amu; and 0.62% of* ^{70}*Zn with an atomic weight of 69.925 amu. Calculate the average atomic weight of Zn.*

Solution

The average atomic weight of zinc $\bar{A}_{\mathrm{Zn}}$ is computed by adding fraction-of-occurrence—atomic weight products for the five isotopes—i.e., using Equation 2.2. (Remember: fraction of occurrence is equal to the percent of occurrence divided by 100.) Thus

$$\bar{A}_{\mathrm{Zn}} = f_{^{64}\mathrm{Zn}} A_{^{64}\mathrm{Zn}} + f_{^{66}\mathrm{Zn}} A_{^{66}\mathrm{Zn}} + f_{^{67}\mathrm{Zn}} A_{^{67}\mathrm{Zn}} + f_{^{68}\mathrm{Zn}} A_{^{68}\mathrm{Zn}} + f_{^{70}\mathrm{Zn}} A_{^{70}\mathrm{Zn}}$$

Including data provided in the problem statement we solve for $\bar{A}_{\mathrm{Zn}}$ as

$$\bar{A}_{\mathrm{Zn}} = (0.4863)(63.929\ \mathrm{amu}) + (0.2790)(65.926\ \mathrm{amu})$$

$$+ (0.0410)(66.927\ \mathrm{amu}) + (0.1875)(67.925\ \mathrm{amu}) + (0.0062)(69.925)$$

$$= 65.400\ \mathrm{amu}$$

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 $(\bar{A}_{\text{In}})$ 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 fracture-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

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

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,

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

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

2.6 *(a) Cite two important quantum-mechanical concepts associated with the Bohr model of the atom.*

(b) Cite two important additional refinements that resulted from the wave-mechanical atomic model.

Solution

(a) Two important quantum-mechanical concepts associated with the Bohr model of the atom are (1) that electrons are particles moving in discrete orbitals, and (2) electron energy is quantized into shells.

(b) Two important refinements resulting from the wave-mechanical atomic model are (1) that electron position is described in terms of a probability distribution, and (2) electron energy is quantized into both shells and subshells--each electron is characterized by four quantum numbers.

2.7 *Relative to electrons and electron states, what does each of the four quantum numbers specify?*

Solution

The n quantum number designates the electron shell.

The l quantum number designates the electron subshell.

The m_l quantum number designates the number of electron states in each electron subshell.

The m_s quantum number designates the spin moment on each electron.

2.8 *Allowed values for the quantum numbers of electrons are as follows:*

$$n = 1, 2, 3, \ldots$$

$$l = 0, 1, 2, 3, \ldots, n-1$$

$$m_l = 0, \pm1, \pm2, \pm3, \ldots, \pm l$$

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

The relationships between n and the shell designations are noted in Table 2.1. Relative to the subshells,

l = 0 corresponds to an s subshell

l = 1 corresponds to a p subshell

l = 2 corresponds to a d subshell

l = 3 corresponds to an f subshell

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* $100(\frac{1}{2})$ *and* $100(-\frac{1}{2})$. *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.*

Answer

For the *L* state, $n = 2$, and eight electron states are possible. Possible l values are 0 and 1, while possible m_l values are 0 and ±1; and possible m_s values are $\pm\frac{1}{2}$. Therefore, for the *s* states, the quantum numbers are $200\left(\frac{1}{2}\right)$ and $200\left(-\frac{1}{2}\right)$. For the *p* states, the quantum numbers are $210(\frac{1}{2})$, $210(-\frac{1}{2})$, $211(\frac{1}{2})$, $211(-\frac{1}{2})$, $21(-1)(\frac{1}{2})$, and $21(-1)(-\frac{1}{2})$.

For the *M* state, $n = 3$, and 18 states are possible. Possible l values are 0, 1, and 2; possible m_l values are 0, ±1, and ±2; and possible m_s values are $\pm\frac{1}{2}$. Therefore, for the *s* states, the quantum numbers are $300(\frac{1}{2})$, $300(-\frac{1}{2})$, for the *p* states they are $310(\frac{1}{2})$, $310(-\frac{1}{2})$, $311(\frac{1}{2})$, $311(-\frac{1}{2})$, $31(-1)(\frac{1}{2})$, and $31(-1)(-\frac{1}{2})$; for the *d* states they are $320(\frac{1}{2})$, $320(-\frac{1}{2})$, $321(\frac{1}{2})$, $321(-\frac{1}{2})$, $32(-1)(\frac{1}{2})$, $32(-1)(-\frac{1}{2})$, $322(\frac{1}{2})$, $322(-\frac{1}{2})$, $32(-2)(\frac{1}{2})$, and $32(-2)(-\frac{1}{2})$.

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 $3p$ and the two $3s$. 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 $3p$. 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 $4s$ and two $5p$. 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 $4p$. 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 $5p$. 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 $4s$. Thus, the electron configuration for a Ni^{2+} ion is $1s^22s^22p^63s^23p^63d^8$.

2.10 *Potassium iodide (KI) exhibits predominantly ionic bonding. The* K^+ *and* I^- *ions have electron structures that are identical to which two inert gases?*

Solution

The K^+ ion is just a potassium atom that has lost one electron; therefore, it has an electron configuration the same as argon (Figure 2.8).

The I^- ion is a iodine atom that has acquired one extra electron; therefore, it has an electron configuration the same as xenon.

2.11 *With regard to electron configuration, what do all the elements in Group IIA of the periodic table have in common?*

Solution

Each of the elements in Group IIA has two *s* electrons.

2.12 *To what group in the periodic table would an element with atomic number 112 belong?*

Solution

From the periodic table (Figure 2.8) the element having atomic number 112 would belong to group IIB. According to Figure 2.8, Ds, having an atomic number of 110 lies below Pt in the periodic table and in the right-most column of group VIII. Moving two columns to the right puts element 112 under Hg and in group IIB.

This element has been artificially created and given the name Copernicium with the symbol Cn. It was named after Nicolaus Copernicus, the Polish scientist who proposed that the earth moves around the sun (and not vice versa).

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.

2.14 *(a) What electron subshell is being filled for the rare earth series of elements on the periodic table?*

(b) What electron subshell is being filled for the actinide series?

Solution

(a) The 4*f* subshell is being filled for the rare earth series of elements.

(b) The 5*f* subshell is being filled for the actinide series of elements.

Bonding Forces and Energies

2.15 Calculate the force of attraction between a Ca^{2+} and an O^{2-} ion whose centers are separated by a distance of 1.25 nm.

Solution

To solve this problem for the force of attraction between these two ions it is necessary to use Equation 2.13, which takes on the form of Equation 2.14 when values of the constants *e* and ε_0 are included—that is

$$F_A = \frac{(2.31 \times 10^{-28} \text{ N-m}^2)\left(|Z_1|\right)\left(|Z_2|\right)}{r^2}$$

If we take ion 1 to be Ca^{2+} and ion 2 to be O^{2-}, then $Z_1 = +2$ and $Z_2 = -2$; also, from the problem statement $r = 1.25$ nm $= 1.25 \times 10^{-9}$ m. Thus, using Equation 2.14, we compute the force of attraction between these two ions as follows:

$$F_A = \frac{(2.31 \times 10^{-28} \text{ N-m}^2)\left(|+2|\right)\left(|-2|\right)}{(1.25 \times 10^{-9} \text{ m})^2}$$

$$5.91 \times 10^{-10} \text{ N}$$

2.16 *The atomic radii of* Mg^{2+} *and* F^{-} *ions are 0.072 and 0.133 nm, respectively.*

(a) 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

This problem is solved in the same manner as Example Problem 2.2.

(a) The force of attraction F_A is calculated using Equation 2.14 taking the interionic separation r to be r_0 the equilibrium separation distance. This value of r_0 is the sum of the atomic radii of the Mg^{2+} and F^{-} ions (per Equation 2.15)—that is

$$r_0 = r_{Mg^{2+}} + r_{F^-}$$

$$= 0.072 \text{ nm} + 0.133 \text{ nm} = 0.205 \text{ nm} = 0.205 \times 10^{-9} \text{ m}$$

We may now compute F_A using Equation 2.14. If was assume that ion 1 is Mg^{2+} and ion 2 is F^{-} then the respective charges on these ions are $Z_1 = Z_{Mg^{2+}} = +2$, whereas $Z_2 = Z_{F^-} = -1$. Therefore, we determine F_A as follows:

$$F_A = \frac{(2.31 \times 10^{-28} \text{ N-m}^2)(|Z_1|)(|Z_2|)}{r_0^2}$$

$$= \frac{(2.31 \times 10^{-28} \text{ N-m}^2)(|+2|)(|-1|)}{(0.205 \times 10^{-9} \text{ m})^2}$$

$$= 1.10 \times 10^{-8} \text{ N}$$

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

$$F_R = -F_A$$

$$= -(1.10 \times 10^{-8} \text{ N}) = -1.10 \times 10^{-8} \text{ N}$$

2.17 *The force of attraction between a divalent cation and a divalent anion is 1.67* $\times$ *10*$^{-8}$ *N. If the ionic radius of the cation is 0.080 nm, what is the anion radius?*

Solution

To begin, let us rewrite Equation 2.15 to read as follows:

$$r_0 = r_{\mathrm{C}} + r_{\mathrm{A}}$$

in which r_{C} and r_{A} represent, respectively, the radii of the cation and anion. Thus, this problem calls for us to determine the value of r_{A}. However, before this is possible, it is necessary to compute the value of r_0 using Equation 2.14, and replacing the parameter *r* with r_0. Solving this expression for r_0 leads to the following:

$$r_0 = \sqrt{\frac{(2.31 \times 10^{-28} \text{ N-m}^2)\left(|Z_{\mathrm{C}}|\right)\left(|Z_{\mathrm{A}}|\right)}{F_A}}$$

Here Z_{C} and Z_{A} represent charges on the cation and anion, respectively. Furthermore, inasmuch as both ion are divalent means that $Z_{\mathrm{C}} = +2$ and $Z_{\mathrm{A}} = -2$. The value of r_0 is determined as follows:

$$r_0 = \sqrt{\frac{(2.31 \times 10^{-28} \text{ N-m}^2)\left(|+2|\right)\left(|-2|\right)}{1.67 \times 10^{-8} \text{ N}}}$$

$$= 0.235 \times 10^{-9} \text{ m} = 0.235 \text{ nm}$$

Using the version of Equation 2.15 given above, and incorporating this value of r_0 and also the value of r_{C} given in the problem statement (0.080 nm) it is possible to solve for r_{A}:

$$r_{\mathrm{A}} = r_0 - r_{\mathrm{C}}$$

$$= 0.235 \text{ nm} - 0.080 \text{ nm} = 0.155 \text{ nm}$$

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,*

$$E_N = -\frac{A}{r} + \frac{B}{r^n} \tag{2.17}$$

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

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

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

(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

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

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

2.19 *For a* Na^+–Cl^- *ion pair, attractive and repulsive energies* E_A *and* E_R, *respectively, depend on the distance between the ions r, according to*

$$E_A = -\frac{1.436}{r}$$

$$E_R = \frac{7.32 \times 10^{-6}}{r^8}$$

For these expressions, energies are expressed in electron volts per Na^+–Cl^- *pair, and r is the distance in nanometers. The net energy* E_N *is just the sum of the preceding two expressions.*

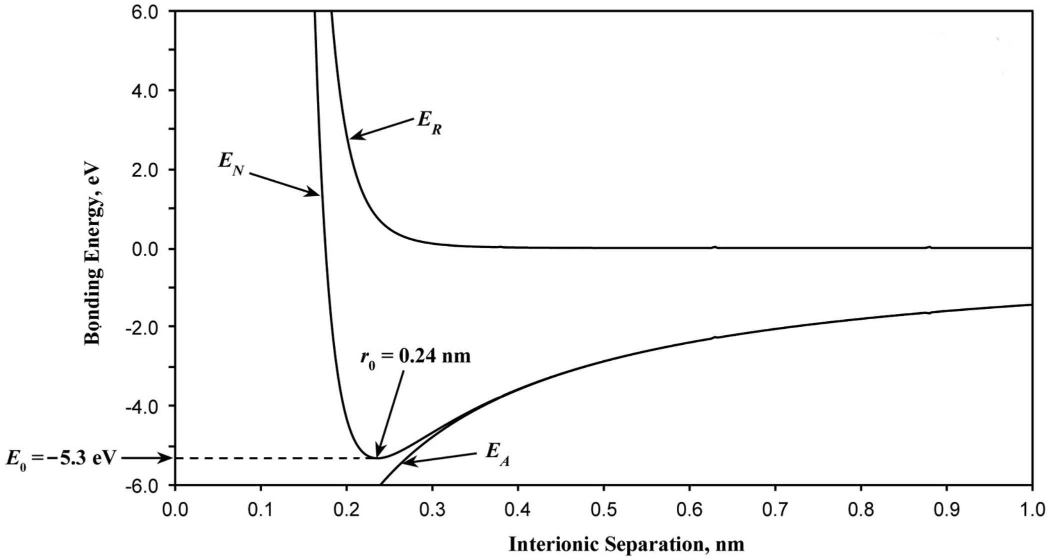
(a) Superimpose on a single plot E_N, E_R, *and* E_A *versus r up to 1.0 nm.*

(b) On the basis of this plot, determine (i) the equilibrium spacing r_0 *between the* Na^+ *and* Cl^- *ions, and (ii) the magnitude of the bonding energy* E_0 *between the two ions.*

(c) Mathematically determine the r_0 *and* E_0 *values using the solutions to Problem 2.18, and compare these with the graphical results from part (b).*

Solution

(a) Curves of E_A, E_R, and E_N are shown on the plot below.



(b) From this plot:

r_0 = 0.24 nm

E_0 = –5.3 eV

(c) From Equation 2.17 for E_N

$$A = 1.436$$

$$B = 7.32 \times 10^{-6}$$

$$n = 8$$

Thus,

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

$$= \left[\frac{1.436}{(8)(7.32 \times 10^{-6})}\right]^{1/(1-8)} = 0.236 \text{ nm}$$

and

$$E_0 = -\frac{1.436}{\left[\dfrac{1.436}{(8)(7.32\times10^{-6})}\right]^{1/(1-8)}} + \frac{7.32\times10^{-6}}{\left[\dfrac{1.436}{(8)(7.32\times10^{-6})}\right]^{8/(1-8)}}$$

$$= -5.32 \text{ eV}$$

2.20 *Consider a hypothetical* $X^+–Y^-$ *ion pair for which the equilibrium interionic spacing and bonding energy values are 0.38 nm and –5.37 eV, respectively. If it is known that n in Equation 2.17 has a value of 8, using the results of Problem 2.18, determine explicit expressions for attractive and repulsive energies* E_A *and* E_R *of Equations 2.9 and 2.11.*

Solution

(a) This problem gives us, for a hypothetical X^+-Y^- ion pair, values for r_0 (0.38 nm), E_0 (– 5.37 eV), and *n* (8), and asks that we determine explicit expressions for attractive and repulsive energies of Equations 2.9 and 2.11. In essence, it is necessary to compute the values of *A* and *B* in these equations. Expressions for r_0 and E_0 in terms of *n*, *A*, and *B* were determined in Problem 2.18, which are as follows:

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

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

Thus, we have two simultaneous equations with two unknowns (viz. *A* and *B*). Upon substitution of values for r_0 and E_0 in terms of *n*, the above two equations become

$$0.38\text{ nm} = \left(\frac{A}{8B}\right)^{1/(1-8)} = \left(\frac{A}{8B}\right)^{-1/7}$$

and

$$-5.37\text{ eV} = -\frac{A}{\left(\frac{A}{8B}\right)^{1/(1-8)}} + \frac{B}{\left(\frac{A}{8B}\right)^{8/(1-8)}}$$

$$= -\frac{A}{\left(\frac{A}{8B}\right)^{-1/7}} + \frac{B}{\left(\frac{A}{10B}\right)^{-8/7}}$$

We now want to solve these two equations simultaneously for values of *A* and *B*. From the first of these two equations, solving for *A*/8*B* leads to

$$\frac{A}{8B} = (0.38\text{ nm})^{-7}$$

Furthermore, from the above equation the A is equal to

$$A = 8B(0.38\text{ nm})^{-7}$$

When the above two expressions for $A/8B$ and A are substituted into the above expression for E_0 (– 5.37 eV), the following results

$$-5.37\text{ eV} = = -\frac{A}{\left(\frac{A}{8B}\right)^{-1/7}} + \frac{B}{\left(\frac{A}{10B}\right)^{-8/7}}$$

$$= -\frac{8B(0.38\text{ nm})^{-7}}{\left[(0.38\text{ nm})^{-7}\right]^{-1/7}} + \frac{B}{\left[(0.38\text{ nm})^{-7}\right]^{-8/7}}$$

$$= -\frac{8B(0.38\text{ nm})^{-7}}{0.38\text{ nm}} + \frac{B}{(0.38\text{ nm})^{8}}$$

Or

$$-5.37\text{ eV} = = -\frac{8B}{(0.38\text{ nm})^{8}} + \frac{B}{(0.38\text{ nm})^{8}} = -\frac{7B}{(0.38\text{ nm})^{8}}$$

Solving for B from this equation yields

$$B = 3.34 \times 10^{-4}\text{ eV-nm}^{8}$$

Furthermore, the value of A is determined from one of the previous equations, as follows:

$$A = 8B(0.38\text{ nm})^{-7} = (8)(3.34 \times 10^{-4}\text{ eV-nm}^{8})(0.38\text{ nm})^{-7}$$

$$= 2.34\text{ eV-nm}$$

Thus, Equations 2.9 and 2.11 become

$$E_A = -\frac{2.34}{r}$$

$$E_R = \frac{3.34 \times 10^{-4}}{r^{8}}$$

Of course these expressions are valid for r and E in units of nanometers and electron volts, respectively.

2.21 *The net potential energy* E_N *between two adjacent ions is sometimes represented by the expression*

$$E_N = -\frac{C}{r} + D\exp\left(-\frac{r}{\rho}\right) \tag{2.18}$$

in which r is the interionic separation and C, D, and ρ are constants whose values depend on the specific material.

(a) Derive an expression for the bonding energy E_0 *in terms of the equilibrium interionic separation* r_0 *and the constants D and ρ using the following procedure:*

(i) Differentiate E_N *with respect to r, and set the resulting expression equal to zero.*

(ii) Solve for C in terms of D, ρ, and r_0.

(iii) Determine the expression for E_0 *by substitution for C in Equation 2.18.*

(b) Derive another expression for E_0 *in terms of* r_0*, C, and ρ using a procedure analogous to the one outlined in part* (a).

Solution

(a) Differentiating Equation 2.18 with respect to *r* yields

$$\frac{dE}{dr} = \frac{d\left(-\frac{C}{r}\right)}{dr} - \frac{d\left[D\exp\left(-\frac{r}{\rho}\right)\right]}{dr}$$

$$= \frac{C}{r^2} - \frac{D\exp\left(-\frac{r}{\rho}\right)}{\rho}$$

At $r = r_0$, $dE/dr = 0$, and

$$\frac{C}{r_0^2} = \frac{D\exp\left(-\frac{r_0}{\rho}\right)}{\rho} \tag{2.18a}$$

Solving for *C* yields

$$C = \frac{r_0^2 D\exp\left(-\frac{r_0}{\rho}\right)}{\rho}$$

Substitution of this expression for C into Equation 2.18 yields an expression for E_0 as

$$E_0 = -\frac{\dfrac{r_0^2 D \exp\left(-\dfrac{r_0}{\rho}\right)}{\rho}}{r_0} + D\exp\left(-\frac{r_0}{\rho}\right)$$

$$= -\frac{r_0 D \exp\left(-\dfrac{r_0}{\rho}\right)}{\rho} + D\exp\left(-\frac{r_0}{\rho}\right)$$

$$= D\left(1 - \frac{r_0}{\rho}\right)\exp\left(-\frac{r_0}{\rho}\right)$$

(b) Now solving for D from Equation 2.18a above yields

$$D = \frac{C\rho \exp\left(\dfrac{r_0}{\rho}\right)}{r_0^2}$$

Substitution of this expression for D into Equation 2.18 yields an expression for E_0 as

$$E_0 = -\frac{C}{r_0} + \left[\frac{C\rho \exp\left(\dfrac{r_0}{\rho}\right)}{r_0^2}\right]\exp\left(-\frac{r_0}{\rho}\right)$$

$$= -\frac{C}{r_0} + \frac{C\rho}{r_0^2}$$

$$E_0 = \frac{C}{r_0}\left(\frac{\rho}{r_0} - 1\right)$$

Primary Interatomic Bonds

2.22 *(a) Briefly cite the main differences among ionic, covalent, and metallic bonding.*

(b) State the Pauli exclusion principle.

Solution

(a) The main differences between the various forms of primary bonding are:

Ionic--there is electrostatic attraction between oppositely charged ions.

Covalent--there is electron sharing between two adjacent atoms such that each atom assumes a stable electron configuration.

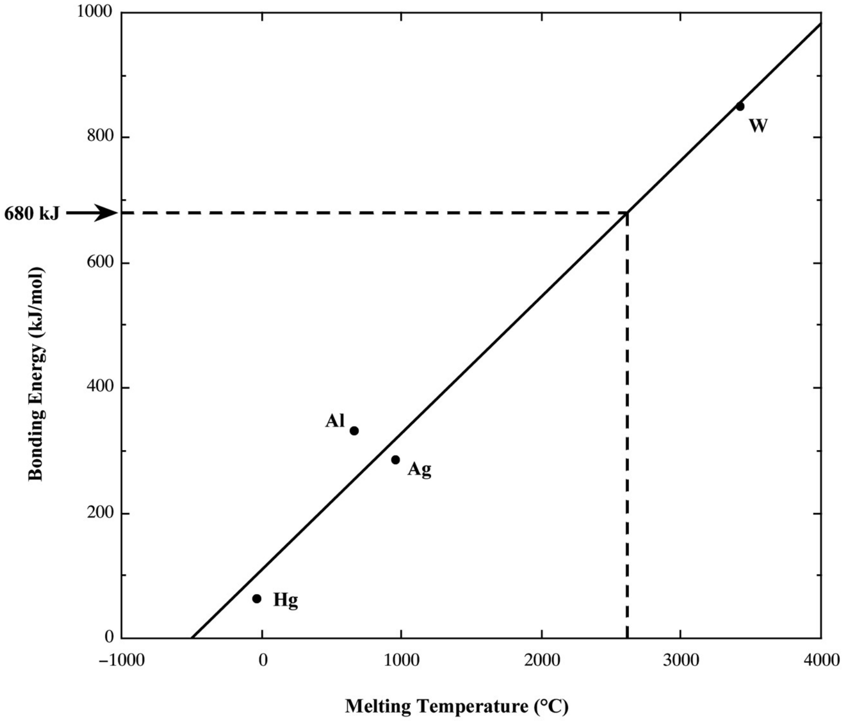
Metallic--the positively charged ion cores are shielded from one another, and also "glued" together by the sea of valence electrons.

(b) The Pauli exclusion principle states that each electron state can hold no more than two electrons, which must have opposite spins.

2.23 *Make a plot of bonding energy versus melting temperature for the metals listed in Table 2.3. Using this plot, approximate the bonding energy for molybdenum, which has a melting temperature of 2617°C.*

Solution

Below is plotted the bonding energy versus melting temperature for these four metals. From this plot, the bonding energy for molybdenum (melting temperature of 2617°C) should be approximately 680 kJ/mol. The experimental value is 660 kJ/mol.



Secondary Bonding or van der Waals Bonding

2.24 *Explain why hydrogen fluoride (HF) has a higher boiling temperature than hydrogen chloride (HCl) (19.4 vs. –85°C), even though HF has a lower molecular weight.*

Solution

The intermolecular bonding for HF is hydrogen, whereas for HCl, the intermolecular bonding is van der Waals. Since the hydrogen bond is stronger than van der Waals, HF will have a higher melting temperature.

Mixed Bonding

2.25 *Compute the %IC of the interatomic bond for each of the following compounds: MgO, GaP, CsF, CdS, and FeO.*

Solution

The percent ionic character is a function of the electron negativities of the ions X_A and X_B according to Equation 2.16. The electronegativities of the elements are found in Figure 2.9.

For MgO, X_{Mg} = 1.3 and X_O = 3.5, and therefore,

$$\%\text{IC} = \left[1 - \exp(-0.25)(3.5 - 1.3)^2\right] \times 100 = 70.1\%$$

For GaP, X_{Ga} = 1.8 and X_P = 2.1, and therefore,

$$\%\text{IC} = \left[1 - \exp(-0.25)(2.1 - 1.8)^2\right] \times 100 = 2.2\%$$

For CsF, X_{Cs} = 0.9 and X_F = 4.1, and therefore,

$$\%\text{IC} = \left[1 - \exp(-0.25)(4.1 - 0.9)^2\right] \times 100 = 92.3\%$$

For CdS, X_{Cd} = 1.5 and X_S = 2.4, and therefore,

$$\%\text{IC} = \left[1 - \exp(-0.25)(2.4 - 1.5)^2\right] \times 100 = 18.3\%$$

For FeO, X_{Fe} = 1.7 and X_O = 3.5, and therefore,

$$\%\text{IC} = \left[1 - \exp(-0.25)(3.5 - 1.7)^2\right] \times 100 = 55.5\%$$

2.26 *(a) Calculate %IC of the interatomic bonds for the intermetallic compound* Al_6Mn. *(b) On the basis of this result what type of interatomic bonding would you expect to be found in* Al_6Mn*?*

Solution

(a) The percent ionic character is a function of the electron negativities of the ions X_A and X_B according to Equation 2.16. The electronegativities for Al and Mn (Figure 2.9) are 1.5 and 1.6, respectively. Therefore the percent ionic character is determined using Equation 2.16 as follows:

$$\%\text{IC} = \left[1 - \exp(-0.25)(1.6-1.5)^2\right] \times 100 = 0.25\%$$

(b) Because the percent ionic character is exceedingly small (0.25%) and this intermetallic compound is composed of two metals, the bonding is completely metallic.

Bonding Type-Material Classification Correlations

2.27 *What type(s) of bonding would be expected for each of the following materials: solid xenon, calcium fluoride (*CaF_2*), bronze, cadmium telluride (CdTe), rubber, and tungsten?*

Solution

For solid xenon, the bonding is van der Waals since xenon is an inert gas.

For CaF_2, the bonding is predominantly ionic (but with some slight covalent character) on the basis of the relative positions of Ca and F in the periodic table.

For bronze, the bonding is metallic since it is a metal alloy (composed of copper and tin).

For CdTe, the bonding is predominantly covalent (with some slight ionic character) on the basis of the relative positions of Cd and Te in the periodic table.

For rubber, the bonding is covalent with some van der Waals. (Rubber is composed primarily of carbon and hydrogen atoms.)

For tungsten, the bonding is metallic since it is a metallic element from the periodic table.

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

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

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

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.

2.2FE *Which of the following electron configurations is for an inert gas?*

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

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

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

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

Solution

The correct answer is A. The $1s^2 2s^2 2p^6 3s^2 3p^6$ electron configuration is that of an inert gas because of filled 3*s* and 3*p* subshells.

2.3FE *What type(s) of bonding would be expected for bronze (a copper-tin alloy)?*

(A) Ionic bonding

(B) Metallic bonding

(C) Covalent bonding with some van der Waals bonding

(D) van der Waals bonding

Solution

The correct answer is B. For bronze, the bonding is metallic because it is a metal alloy.

2.4FE *What type(s) of bonding would be expected for rubber?*

(A) Ionic bonding

(B) Metallic bonding

(C) Covalent bonding with some van der Waals bonding

(D) van der Waals bonding

Solution

The correct answer is C. For rubber, the bonding is covalent with some van der Waals bonding. (Rubber is composed primarily of carbon and hydrogen atoms.)