

CHAPTER 2

ATOMIC STRUCTURE AND INTERATOMIC BONDING

PROBLEM SOLUTIONS

2.2 Chromium has four naturally-occurring isotopes: 4.34% of ^{50}Cr , with an atomic weight of 49.9460 amu, 83.79% of ^{52}Cr , with an atomic weight of 51.9405 amu, 9.50% of ^{53}Cr , with an atomic weight of 52.9407 amu, and 2.37% of ^{54}Cr , with an atomic weight of 53.9389 amu. On the basis of these data, confirm that the average atomic weight of Cr is 51.9963 amu.

Solution

The average atomic weight of chromium (\bar{A}_{Cr}) is computed by adding fraction-of-occurrence/atomic weight products for the four isotopes. Thus

$$\begin{aligned}\bar{A}_{\text{Cr}} &= f_{50\text{Cr}} A_{50\text{Cr}} + f_{52\text{Cr}} A_{52\text{Cr}} + f_{53\text{Cr}} A_{53\text{Cr}} + f_{54\text{Cr}} A_{54\text{Cr}} \\ &= (0.0434)(49.9460 \text{ amu}) + (0.8379)(51.9405 \text{ amu}) + (0.0950)(52.9407 \text{ amu}) \\ &\quad + (0.0237)(53.9389 \text{ amu}) = 51.9963 \text{ amu}\end{aligned}$$

2.5 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.

2.7 Give the electron configurations for the following ions: Fe^{2+} , Al^{3+} , Cu^+ , Ba^{2+} , Br^- , O^{2-} , Fe^{3+} and S^{2-} .

Solution

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

Fe^{2+} : From Table 2.2, the electron configuration for an atom of iron is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$. 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 an Fe^{2+} ion is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$.

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

Cu^+ : From Table 2.2, the electron configuration for an atom of copper is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$. In order to become an ion with a plus one charge, it must lose one electron—in this case the 4s. Thus, the electron configuration for a Cu^+ ion is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$.

Ba^{2+} : The atomic number for barium is 56 (Figure 2.6), and inasmuch as it is not a transition element the electron configuration for one of its atoms is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6 6s^2$. In order to become an ion with a plus two charge, it must lose two electrons—in this case two the 6s. Thus, the electron configuration for a Ba^{2+} ion is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6$.

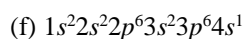
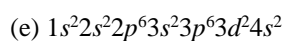
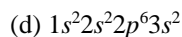
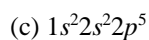
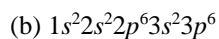
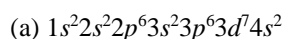
Br^- : From Table 2.2, the electron configuration for an atom of bromine is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$. In order to become an ion with a minus one charge, it must acquire one electron—in this case another 4p. Thus, the electron configuration for a Br^- ion is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$.

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

Fe^{3+} : From Table 2.2, the electron configuration for an atom of iron is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2$. In order to become an ion with a plus three charge, it must lose three electrons—in this case the two 4s and one 3d. Thus, the electron configuration for an Fe^{3+} ion is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$.

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

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



Solution

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

(b) The $1s^2 2s^2 2p^6 3s^2 3p^6$ electron configuration is that of an inert gas because of filled $3s$ and $3p$ subshells.

(c) The $1s^2 2s^2 2p^5$ electron configuration is that of a halogen because it is one electron deficient from having a filled L shell.

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

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

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

2.13 Calculate the force of attraction between a K^+ and an O^{2-} ion the centers of which are separated by a distance of 1.6 nm.

Solution

The attractive force between two ions F_A is just the derivative with respect to the interatomic separation of the attractive energy expression, Equation 2.9, which is just

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

The constant A in this expression is defined in Equation 2.10. Since the valences of the K^+ and O^{2-} ions (Z_1 and Z_2) are +1 and -2, respectively, $Z_1 = 1$ and $Z_2 = 2$, then

$$\begin{aligned} F_A &= \frac{(Z_1 e)(Z_2 e)}{4\pi\epsilon_0 r^2} \\ &= \frac{(1)(2)(1.602 \times 10^{-19} \text{ C})^2}{(4)(\pi)(8.85 \times 10^{-12} \text{ F/m})(1.6 \times 10^{-9} \text{ m})^2} \\ &= 1.8 \times 10^{-10} \text{ N} \end{aligned}$$

2.14 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,

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

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

$$\begin{aligned}\frac{dE_N}{dr} &= \frac{d}{dr} \left(-\frac{A}{r} \right) + \frac{d}{dr} \left(\frac{B}{r^n} \right) \\ &= \frac{A}{r^2} - \frac{nB}{r^{n+1}} = 0\end{aligned}$$

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

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

or

$$r_0 = \sqrt[n]{\frac{A}{nB}}$$

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

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

2.16 Consider a hypothetical X^+-Y^- ion pair for which the equilibrium interionic spacing and bonding energy values are 0.38 nm and -6.13 eV, respectively. If it is known that n in Equation 2.17 has a value of 10, using the results of Problem 2.14, determine explicit expressions for attractive and repulsive energies E_A and E_R of Equations 2.9 and 2.11.

Solution

This problem gives us, for a hypothetical X^+-Y^- ion pair, values for r_0 (0.38 nm), E_0 (-6.13 eV), and n (10), 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 2.14, 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 , these equations take the forms

$$0.38 \text{ nm} = \left(\frac{A}{10B} \right)^{1/(1-10)} = \left(\frac{A}{10B} \right)^{-1/9}$$

and

$$\begin{aligned} -6.13 \text{ eV} &= - \frac{A}{\left(\frac{A}{10B} \right)^{1/(1-10)}} + \frac{B}{\left(\frac{A}{10B} \right)^{10/(1-10)}} \\ &= - \frac{A}{\left(\frac{A}{10B} \right)^{-1/9}} + \frac{B}{\left(\frac{A}{10B} \right)^{-10/9}} \end{aligned}$$

We now want to solve these two equations simultaneously for values of A and B . From the first of these two equations, solving for $A/10B$ leads to

$$\frac{A}{10B} = (0.38 \text{ nm})^{-9}$$

Furthermore, from the above equation the A is equal to

$$A = 10B(0.38 \text{ nm})^{-9}$$

When the above two expressions for $A/10B$ and A are substituted into the above expression for E_0 (-6.13 eV), the following results

$$\begin{aligned} -6.13 \text{ eV} &= -\frac{A}{10B} + \frac{B}{A} \\ &= -\frac{10B(0.38 \text{ nm})^{-9}}{10B} + \frac{B}{10B(0.38 \text{ nm})^{-9}} \\ &= -\frac{10B(0.38 \text{ nm})^{-9}}{0.38 \text{ nm}} + \frac{B}{(0.38 \text{ nm})^{10}} \end{aligned}$$

or

$$-6.13 \text{ eV} = -\frac{10B}{(0.38 \text{ nm})^{10}} + \frac{B}{(0.38 \text{ nm})^{10}} = -\frac{9B}{(0.38 \text{ nm})^{10}}$$

Solving for B from this equation yields

$$B = 4.28 \times 10^{-5} \text{ eV-nm}^{10}$$

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

$$\begin{aligned} A &= 10B(0.38 \text{ nm})^{-9} = (10)(4.28 \times 10^{-5} \text{ eV-nm}^{10})(0.38 \text{ nm})^{-9} \\ &= 2.59 \text{ eV-nm} \end{aligned}$$

Thus, Equations 2.9 and 2.11 become

$$\begin{aligned} E_A &= -\frac{2.59}{r} \\ E_R &= \frac{4.28 \times 10^{-5}}{r^{10}} \end{aligned}$$

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

- 2.18 (a) Briefly cite the main differences between 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.

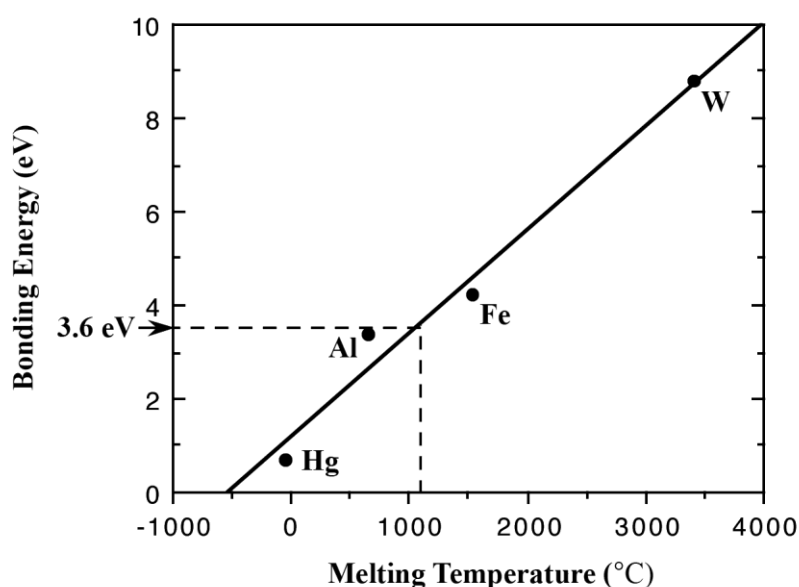
Metallic—the positively charged ion cores are shielded from one another, and also "glued" together by the sea of valence electrons.

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

- 2.19 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 copper, which has a melting temperature of 1084°C.

Solution

Below is plotted the bonding energy versus melting temperature for these four metals. From this plot, the bonding energy for copper (melting temperature of 1084°C) should be approximately 3.6 eV. The experimental value is 3.5 eV.



2.20 Using Table 2.2, determine the number of covalent bonds that are possible for atoms of the following elements: germanium, phosphorus, selenium, and chlorine.

Solution

For germanium, having the valence electron structure $4s^24p^2$, $N' = 4$; thus, there are $8 - N' = 4$ covalent bonds per atom.

For phosphorus, having the valence electron structure $3s^23p^3$, $N' = 5$; thus, there is $8 - N' = 3$ covalent bonds per atom.

For selenium, having the valence electron structure $4s^24p^4$, $N' = 6$; thus, there are $8 - N' = 2$ covalent bonds per atom.

For chlorine, having the valence electron structure $3s^23p^5$, $N' = 7$; thus, there are $8 - N' = 1$ covalent bond per atom.