Name: 陈稼霖
StudentID: 45875852

Problem 21.12. Compute the volume (in cubic angstroms) of the unit cell of potassium hexacyanoferrate(III) ($K_3Fe(CN)_6$), a substance that crystallizes in the monoclinic system with $a = 8.40$ Å, $b = 10.44$ Å, and $c = 7.04$ Åand with $\beta = 107.5°$.

Solution: The volume of the unit cell of $K_3Fe(CN)_6$ is

$$V = abc\sin\beta = 0.840nm \times 1.044nm \times 0.704nm \times \sin 107.5° = 0.589nm^3$$

□

Problem 21.22. The structure of aluminum is fcc and its density is $\rho = 2.70$ g cm^{-3}.
(a) How many Al atoms belong to a unit cell?
(b) Calculate a, the lattice parameter, and d, the nearest neighbor distance.

Solution:
(a) $8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$ Al atoms belongs to a unit cell.
(b) The density of Al is given by

$$\rho = \frac{M(Al)}{\frac{N_a}{4}a^3}$$
$$\Longrightarrow 2.70 \times 10^3 kg\ m^{-3} = \frac{27.0 \times 10^{-3} kg\ mol^{-1}}{\frac{6.02\times10^{23} mol^{-1}}{4}a^3}$$

Therefore, the lattice parameter is

$$\Longrightarrow a = 4.05 \times 10^{10} m = \underline{4.05Å}$$

The nearest neighbor distance is

$$d = \frac{\sqrt{2}}{2}a = \underline{2.86Å}$$

□

Problem 21.28. Classify each of the following solids as molecular, ionic, metallic, or covalent.
(a) Rb (b) C_5H_{12}
(c) B (d) Na_2HPO_4

Solution:
(a) Rb is metallic.
(b) C_5H_{12} is molecular.
(c) B is covalent.
(d) Na_2HPO_4 is ionic.

□

Problem 21.34. Repeat the determinations of the preceding problem for the NaCl crystal, referring to Figure 21.16.

Solution:
The number of nearest neighbors of a Na+ ion in crystalline NaCl is 6.
The number of second nearest neighbors is 12.
The number of third nearest neighbors is 8.
The nearest neighbors of the Na^+ are Cl^- ions.
The second nearest neighbors are Na^+ ions. □

Problem 21.40. Repeat the calculation of problem 39 for CsCl, taking the Madelung constant from Table 21.5 and taking the radii of Cs^+ and Cl_2 to be 1.67 Åand 1.81 Å.

Solution: The lattice energy is

$$\begin{aligned}\text{Lattice Energy} =&(1-10\%)\frac{N_A e^2 M}{4\pi\epsilon_0 R_0}\\=&(1-10\%)\frac{6.02\times10^{23}mol^{-1}\times(1.602\times10^{-19}C)^2\times1.7627}{4\times8.854\times10^{-12}C^2\ J^{-1}\ m^{-1}\times(1.67+1.81)\times10^{-10}m}\\=&633kJ\ mol^{-1}\end{aligned}$$

Therefore, the energy needed to dissociate 1.00 mol of crystalline CsCl into its gaseous ions is $633kJ$. □

Problem 21.45. The number of beams diffracted by a single crystal depends on the wavelength l of the X-rays used and on the volume associated with one lattice point in the crystal – that is, on the volume V_p of a primitive unit cell. An approximate formula is

$$\text{number of diffracted beams} = \frac{4}{3}\pi(\frac{2}{\lambda})^3 V_p$$

(a) Compute the volume of the conventional unit cell of crystalline sodium chloride. This cell is cubic and has an edge length of 5.6402 Å.
(b) The NaCl unit cell contains four lattice points. Compute the volume of a primitive unit cell for NaCl.
(c) Use the formula given in this problem to estimate the number of diffracted rays that will be observed if NaCl is irradiated with X-rays of wavelength 2.2896 Å.
(d) Use the formula to estimate the number of diffracted rays that will be observed if NaCl is irradiated with X-rays having the shorter wavelength 0.7093 Å.

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Solution:

(a) The volume of the conventional unit cell of crystalline sodium chloride is

$$V = a^3 = (0.56402nm)^3 = \underline{0.17943nm^3}$$

(b) The volume of a primitive unit cell for NaCl is

$$V_p = \frac{V}{4} = \frac{0.17943nm^3}{4} = \underline{0.04486nm^3}$$

(c) If the X-rays have wavelength of 2.2896 Å, the number of diffracted rays is

$$\text{number of diffracted beams} = \frac{4}{3}\pi(\frac{2}{\lambda})^3 V_p = \frac{4}{3}\pi \times (\frac{2}{0.22896nm})^3 \times 0.04486nm^3 = \underline{125}$$

(d) If the X-rays have wavelength of $0.07093nm$, the number of diffracted rays is

$$\text{number of diffracted beams} = \frac{4}{3}\pi(\frac{2}{\lambda})^3 V_p = \frac{4}{3}\pi \times (\frac{2}{0.07093nm})^3 \times 0.04486nm^3 = \underline{4211}$$

□