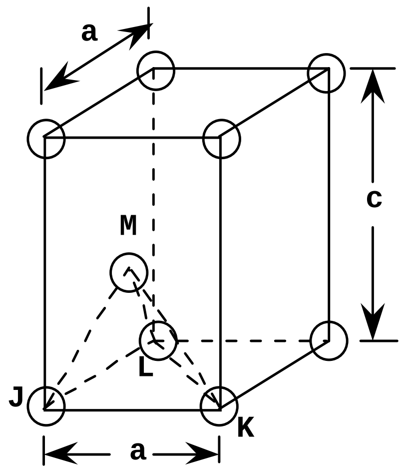
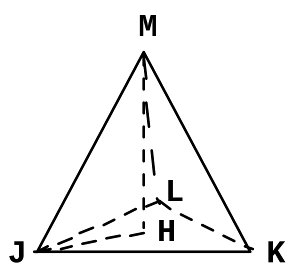
MATSE 259
Solutions to homework #2

1. For the HCP crystal structure, show that the ideal c/a ratio is 1.633.

We are asked to show that the ideal **c**/**a** ratio for HCP is 1.633. A sketch of one third of an HCP unit cell is shown below.



Consider the tetrahedron labeled as **JKLM**, which is reconstructed as



The atom at point **M** is midway between the top and bottom faces of the unit cell that is $\overline{\mathbf{MH}}$ = **c**/2. And, since atoms at points **J**, **K**, and **M**, all touch one another,

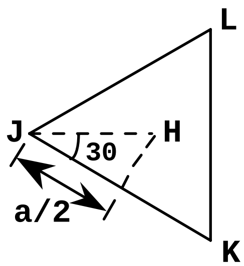
$$\overline{JM} = \overline{JK} = 2R = a$$

where **R** is the atomic radius. Furthermore, from triangle **JHM**,

$$(\overline{JM})^2 = (\overline{JH})^2 + (\overline{MH})^2, \text{ or}$$

$$a^2 = (\overline{JH})^2 + \left(\frac{c}{2}\right)^2$$

Now, we can determine the $\overline{\mathbf{JH}}$ length by consideration of triangle **JKL**, which is an equilateral triangle,



$$\cos 30^\circ = \frac{a/2}{JH} = \frac{\sqrt{3}}{2}, \text{ and}$$

$$\overline{JH} = \frac{a}{\sqrt{3}}$$

Substituting this value for $\overline{\mathbf{JH}}$ in the above expression yields

$$a^2 = \left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 = \frac{a^2}{3} + \frac{c^2}{4}$$

and, solving for **c**/**a**

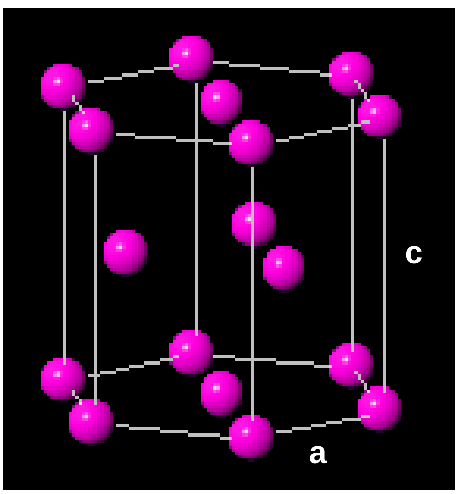
$$\frac{c}{a} = \sqrt{\frac{8}{3}} = 1.633$$

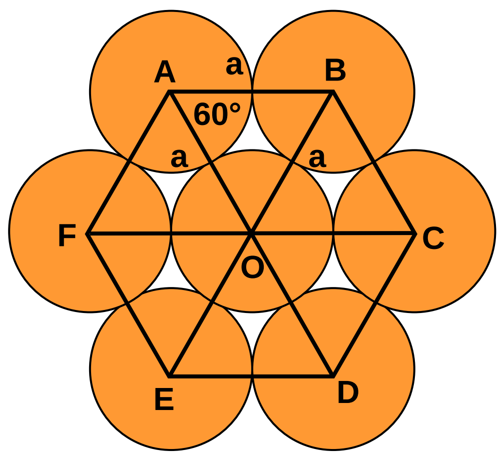
2. Show that the atomic packing factor for HCP is 0.74.

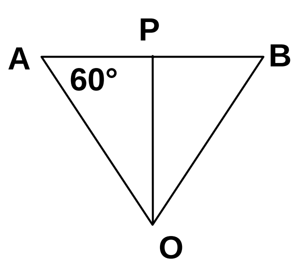
This problem calls for a demonstration that the **APF** for HCP is 0.74. Again, the **APF** is the ratio of the total sphere volume, V_S, to the unit cell volume, V_C. For HCP, there are the equivalent of six spheres per unit cell, and thus

$$V_S = 6\left(\frac{4\pi R^3}{3}\right) = 8\pi R^3$$

Now, the unit cell volume is the product of the base area times the cell height, **c**. The base area can be calculated as follows. The following figure shows an HCP unit cell and the basal plane. The base area is equal to six times the area of the equilateral triangle, OAB.







The area of equilateral triangle, OAB = $0.5 \times AB \times OP$

$$= \tfrac{1}{2} \times AB \times AO \sin 60°$$

$$= \tfrac{1}{2} \times \mathbf{a} \times \mathbf{a} \sin 60° = \frac{\sqrt{3}}{4} a^2$$

Thus, the area of the basal plane = 6 × $\frac{\sqrt{3}}{4}\mathbf{a}^2 = \frac{3\sqrt{3}}{2}\mathbf{a}^2$.

Further, as can be seen from the figure of the basal plane, **a** = 2**R**. Therefore, the base area = $6\mathbf{R}^2\sqrt{3}$

Now, using the result of Problem 1, given above, the relation between the unit cell height, **c**, and the basal plane edge length, **a**, is given as:

$$\frac{c}{a} = 1.63$$

Thus, c = 1.63a = 3.26R

The unit cell volume can now be calculated as:

$$V_C = c \times \text{base area} = 3.26R \times 10.392R^2 = 33.878R^3$$

$$\text{Thus, } APF = \frac{V_S}{V_C} = \frac{8\pi R^3}{33.878R^3} = 0.74$$

3. Rhenium has an HCP crystal structure, an atomic radius of 0.137 nm, and a c/a ratio of 1.615. Compute the volume of the unit cell for Re.

This problem asks that we calculate the unit cell volume, V_C, for Re which has an HCP crystal structure. Now, $\mathbf{V_C}$ = **c** × base area, and the base area has been calculated in Problem 2 above as $6\mathbf{R}^2\sqrt{3}$. Thus,

$$VC = c \times 6R^2\sqrt{3}$$

In this problem, **c** = 1.615**a**, and **a** = 2**R**. Therefore

$$V_C = 1.615 \times 2 \times 6\sqrt{3} \times R^3$$

$$= 1.615 \times 2 \times 6\sqrt{3} \times (1.37 \text{ x } 10^{-8} \text{ cm})^3 = 8.63 \text{ x } 10^{-23} \text{ cm}^3 = 8.63 \text{ x } 10^{-2} \text{ nm}^3$$