Graded problems:

1. The values of the ionic radii assigned to Ti^{4+} and O_2^- by Pauling are 0.6 and 1.40 Å. What are the values that you would predict for the coordination number of these ions in the structure of TiO_2?

2. The ionic radii listed by Shannon and Prewitt for Zn^{2+} and S^{2-}, when both are in 4-fold coordination, are 0.60 and 1.84 Å.

   a. Compute the lattice constant, *a*, for the cubic form of *ZnS* in which the *S* ions are arranged in face-centered cubic packing and *Zn* ions occupy half of the available tetrahedral interstices.
   b. What is the size of the largest cation that could fit into the unoccupied octahedral site without distortion of the array of ions?

3. Compute the fraction of available volume (that is, total volume of spheres divided by the volume of the unit cell) that is occupied by spheres arranged in:

   a. Simple cubic packing
   b. Face-centered cubic packing
   c. Body-centered cubic packing

4. For each statement below, identify the type of thermodynamic system and process involved.

   (a) A mole of hydrogen gas is maintained at a constant temperature inside a rigid container impermeable to the gas.

   (b) A system composed of a bar of nickel fused to a bar of gold is maintained at a constant temperature inside an oven at 0.1 atm pressure; Au and Ni diffuse at the junction between the two bars.

(c) The liquid solvent acetone is mixed with liquid nitrogen in a sealed dewar (a container for low-temperature liquids) which is thermally insulated to prevent heat transfer.

(d) A beaker of water is warmed in the sun on your porch.

5. Calculate the total amount of heat absorbed by a mole of neon gas if it undergoes a reversible expansion from 1L to 4L at a constant temperature of 400K, assuming that neon behaves as an ideal gas and the internal energy of the gas remains constant. What is the entropy change in the gas due to this process?

Problems for additional practice:

6. Another geometry, other than octahedral, that provides 6-fold coordination for a central ion is a triangular prismatic arrangement.

   a. Compute the lower limit that is permitted to the radius ratio of the central ion to that of the surrounding spheres.

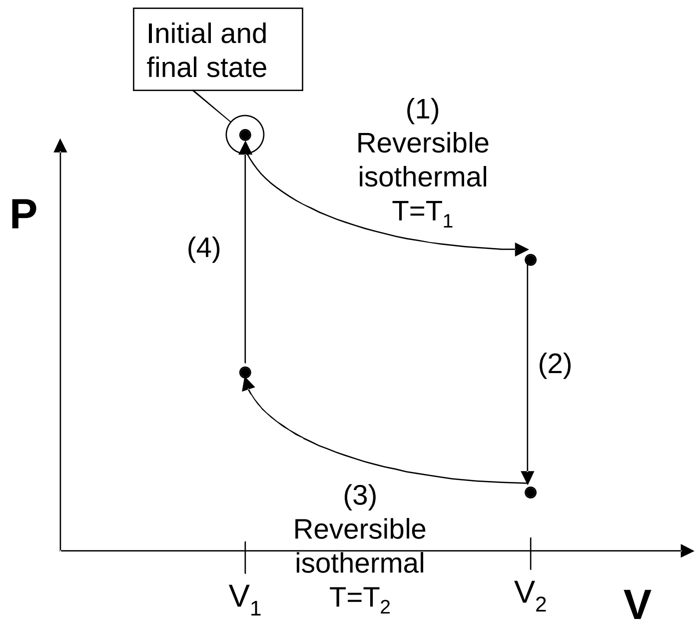
   b. This coordination does appear in structures but is far less common than octahedral coordination. Why?

7. Consider a structure in which four *B* ions surround a central *A* ion. In a tetrahedral arrangement, this configuration for an isolated tetrahedron can be formed for a radius ratio R_A/R_B that is arbitrarily large. Suppose, however, that we would like to build a structure in which these tetrahedral share faces. Is there a radius ratio for which this would be impossible because the interior A spheres pokes out of the face of the tetrahedron?

8. Determine the coordinates of the four tetrahedrally-coordinated interstices that exist within the unit cell of a hexagonal close-packed array of spheres.

9. A system is comprised of 10 g of Ar gas at 0°C and P = 1 atm. When 3400 J of heat are added to the system at constant pressure and temperature, the resultant reversible expansion causes the system to perform 900 J of work. Calculate (a) the initial state (P, V, T), (b) the final state (P, V, T), and (c) ΔU for the process, if the gas is assumed ideal.

10. Determine the total internal energy change and net heat transferred to one mole of an ideal gas undergoing the 4-step process shown schematically below, in terms of T_1, T_2, V_1, and V_2.



11. Many gases do not obey the ideal gas law, but are better described by another equation of state, known as the Van der Waals equation of state:

$$\left(P + \frac{an^2}{V^2}\right)(V - nb) = nRT$$

Carbon dioxide is described by the Van der Waals equation of state, with parameters $a = 0.3640$ (Pa m^6 $mole^{-2}$) and $b = 4.267x10^{-5}$ (m^3 $mole^{-1}$). Compare the work needed to reversibly compress 1 mole of carbon dioxide from 6 L to 2L at a constant temperature of 298 K using the ideal gas model vs. the Van der Waals equation of state.