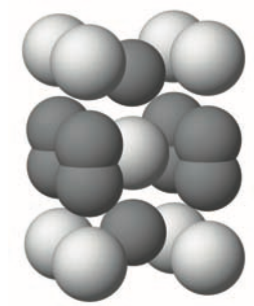
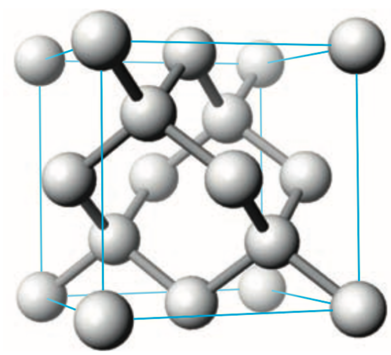
Problems Chapter 12 (Solids)

1. The unit cell shown here is for calcium carbide. How many calcium atoms and how many carbon atoms are in each unit cell? What is the formula of calcium carbide? (Calcium ions are silver in color and carbon atoms are gray.)



2. The solid structure of silicon is shown below.
   a. Describe this crystal as PC, BCC or FCC. What type of holes are occupied in the lattice?
   b. Calculate the density of silicon in g cm^{-3} (given that the cube edge has a length of 543.1 pm).



3. Sodium metal adopts a body-centered cubic structure with a density of 0.97 g/cm^3. Use this information to estimate the atomic radius of sodium.

4. Vanadium metal has a density of 6.11 g/cm^3. Assuming the vanadium atomic radius is 132 pm, is the vanadium unit cell primitive cubic, body-centered cubic or face-centered cubic?

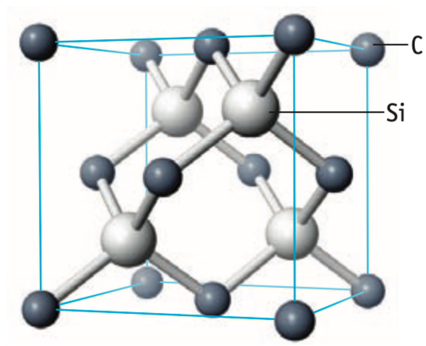
5. Rationalize why chalk (calcium carbonate) has a higher melting point that motor oil (large compounds made of C and H), which has a higher melting point than water, which engages in relatively strong hydrogen-bonding interactions.

6. For each of the following pairs of semiconductors, which one will have the larger band gap: (a) CdS or CdTe? (b) GaN or InP? (c) GaAs or InAs?

7. The melting point of a fictional substance X is 225 ˚C at 10.0 atm. If the density of the solid phase of X is 2.67 g/cm^3 and the density of the liquid phase is 2.78 g/cm^3 at 10.0 atm, predict whether the normal melting point of X will be less than, equal to, or greater than 225 ˚C. Explain.

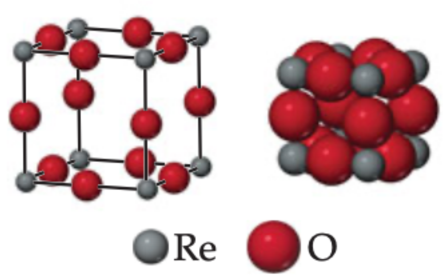
8. Consider the following data for xenon:
   Triple point: –121 ˚C, 280 torr
   Normal melting point: –112 ˚C
   Normal boiling point: –107 ˚C
   What is more dense, Xe (s) or Xe (l)?

9. The solid state structure of silicon carbide, SiC, is shown below. Knowing that the Si–C bond length is 188.8 pm (and the Si–C–Si bond angle is 109.5˚), calculate the density of SiC.



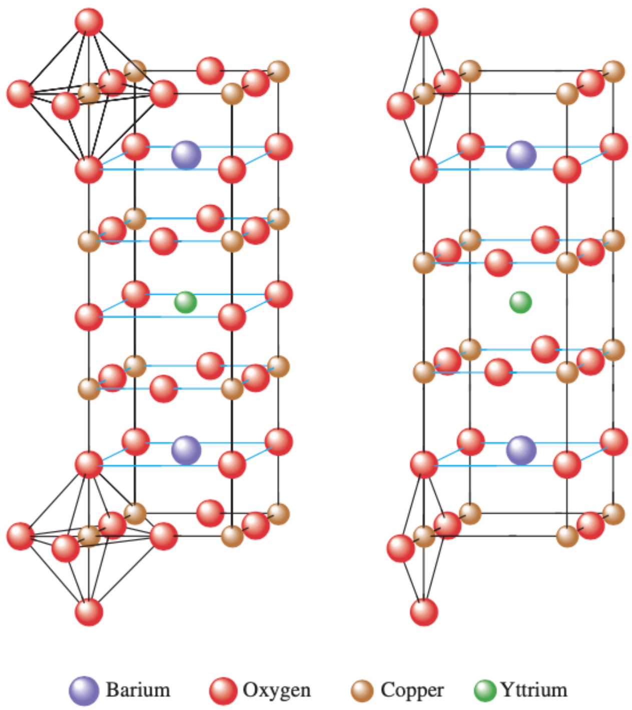
Unit cell of SiC.

10. Rhenium oxide crystallizes with a structure that has a primitive cubic lattice, as shown here. In the image on the left, the sizes of the ions have been reduced to show the entire unit cell.



   a. How many atoms of each type are there per unit cell?
   b. Use the ionic radii of rhenium (0.70 Å) and oxygen (1.26 Å) to estimate the length of the edge of the unit cell (1 Å = 10^{-10} m).
   c. Use your answers to parts (a) and (b) to estimate the density of this compound.

11. Materials containing the elements Y, Ba, Cu and O that are superconductors (electrical resistance equals zero) at temperatures above that of liquid nitrogen were recently discovered. The structures of these materials are based on the perovskite structure. Were they to have the ideal perovskite structure, the superconductor would have the structure shown in part (a) of the figure. These materials, however, do not act as superconductors unless they are deficient in oxygen. The structure of the actual superconducting phase appears to be that shown in part (b) of the figure.
    a. What is the formula of this ideal perovskite material?
    b. What is the formula of the actual superconductor?



(a) Ideal perovskite structure

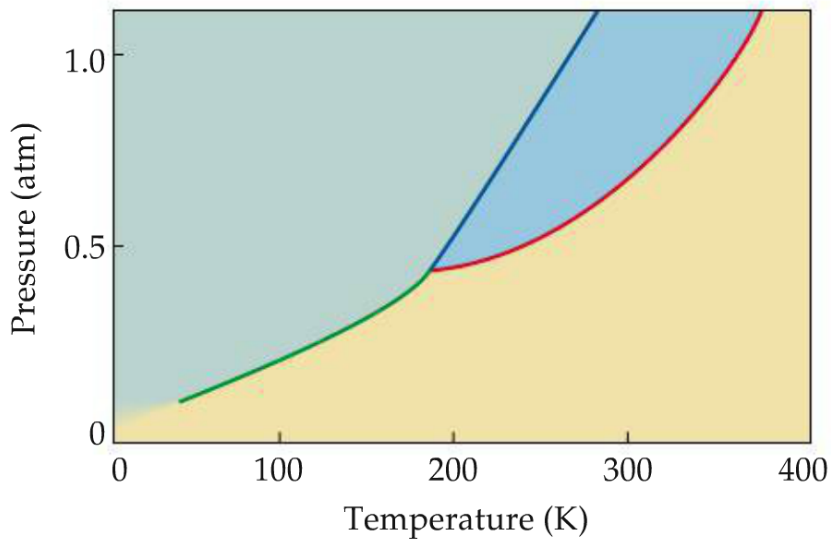
(b) Actual structure of superconductor

12. If you wanted to dope GaAs to make a n-type semiconductor with an element to replace Ga, which element(s) would you pick?

13. Using the thermochemical data below and an estimated value of –2481 kJ/mol for the lattice enthalpy for Na_2O, calculate the value for the second electron affinity of oxygen [O^- (g) + e– (g) → O^{2-} (g)].

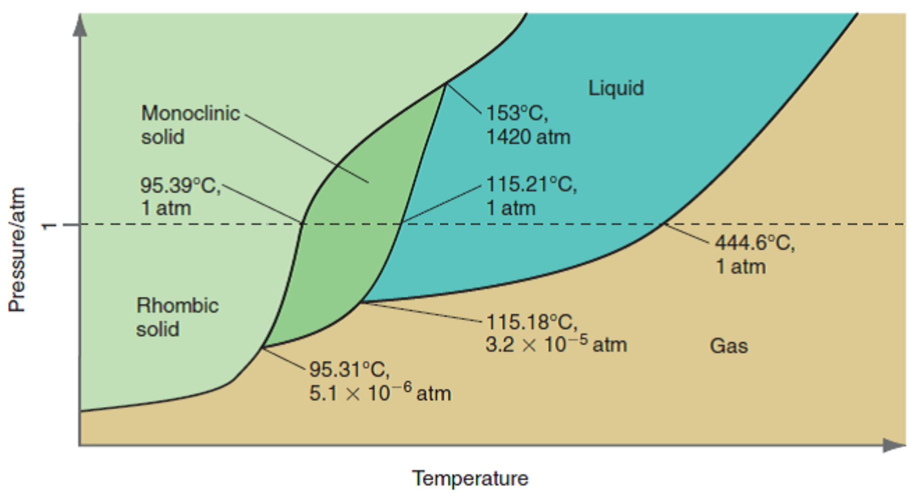
Quantity	Numerical Value (kJ/mol)
Enthalpy of atomization of Na	107.3
Ionization energy of Na	495.9
Enthalpy of formation of solid Na_2O	−418.0
Enthalpy of formation of O(g) from O_2	249.1
First electron attachment enthalpy of O	−141.0

14. The phase diagram of a hypothetical substance is shown below.



a. Estimate the normal boiling point and freezing point of the substance.
b. What is the physical state of the substance under the following conditions? (i) T = 150 K, P = 0.2 atm; (ii) T = 100 K, P = 0.8 atm; (iii) T = 300 K, P = 1.0 atm
c. What is the triple point of the substance?

15. Use the accompanying phase diagram for sulfur to answer the following questions (the phase diagram is not to scale)



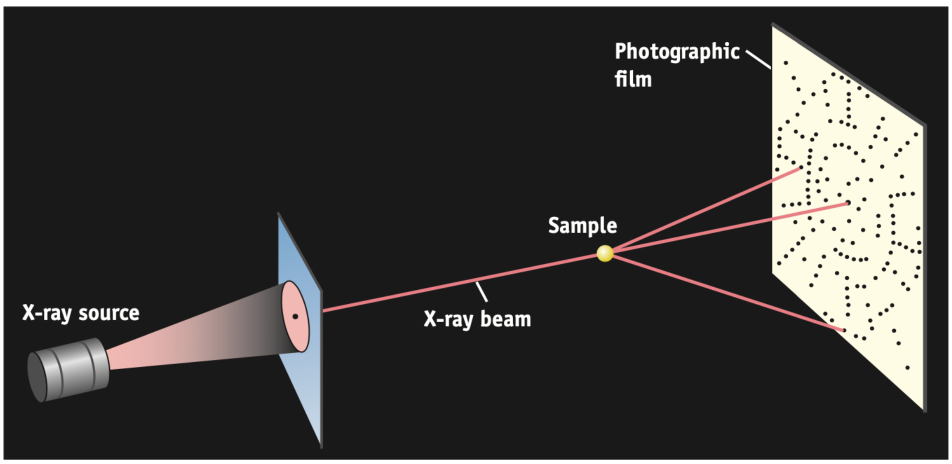
a. How many triple points are in the phase diagram?
b. What phases are in equilibrium at each of the triple points?
c. What phase is stable at 1.0 atm and room temperature?
d. Can monoclinic sulfur exist in equilibrium with sulfur vapor?
e. What are the normal melting point and normal boiling point of sulfur?
f. At a pressure of 1.0 x 10^{-5} atm, can rhombic sulfur sublime?
g. What phase changes occur when the pressure of a sample of sulfur at 100. ˚C is increased from 1.0 x 10^{-8} atm to 1500 atm?

16. Consider the following data concerning four different substances. Label the four substances as either ionic, network, metallic or molecular solids.

Compound	Conducts Electricity as a Solid	Other Properties
B_2H_6	no	gas at 25°C
SiO_2	no	high mp
CsI	no	aqueous solution conducts electricity
W	yes	high mp

Dorothy Mary Crowfoot Hodgkin: the mother of X-ray crystallography or biologically relevant molecules

Crystalline solids are made of a regular pattern of particles arranged into unit cells. Knowledge about the structure of various crystalline solids has been made possible through x-ray crystallography. In an x-ray crystallography experiment, x-rays are directed towards a sample of a substance. These x-rays are scattered by the atoms comprising the substance; the resulting pattern is related to the location of the atoms and ions making up the crystal (the crystal structure is solved).



Solving structures of biologically relevant molecules is often an arduous task. Many of these substances are notoriously difficult to obtain in crystalline form and the molecules comprising them are often very large, containing an intricate pattern of atoms. Dorothy Hodgkin, a British chemist, was a pioneer in this field. Attending grammar school in the 1920s, she had to petition to be allowed to take chemistry instead of domestic science and was one of only two women in her chemistry class. She pursued her PhD in Cambridge University, researching applications of x-ray crystallography in determining the structure of steroids, and was not deterred from her work by a diagnosis of chronic rheumatoid arthritis which she received at the age of just 24. Dorothy Hodgkin solved the structures of multiple molecules of utmost biological importance, such as penicillin, insulin (which took her 35 years!) and vitamin B_{12}. For her latter accomplishment, she was awarded a Nobel Prize in chemistry in 1964, becoming the third woman to ever win a Nobel Prize and the only British woman scientist to win a Nobel Prize in a scientific discipline.

References:

https://www.famousscientists.org/dorothy-hodgkin/ (accessed Feb 8, 2021)
En.wikipedia.org. [online] *Dorothy Hodgkin.* https://en.wikipedia.org/wiki/Dorothy_Hodgkin (accessed Feb 8, 2021)
https://www.nobelprize.org/womenwhochangedscience/stories/dorothy-hodgkin (accessed Feb 8, 2021)