Worksheet 8

March 4th, 2022

Collaborations are encouraged and students must report all collaborators on each assignment. All external sources (websites, books) must be cited. An *extra credit* (*EC*) problem will be available per assignment. Please submit a completed homework on-time to receive *EC* and no partial *EC* (all parts must be correct) will be given out. Additional problems are listed at the end of each assignment. This week's assignment is due *Tuesday, March 8th at 2:00pm.*

1. (5 pts) **Phase Diagram** The phase diagram for carbon is shown in Fig. 1. Answer the following questions:

(a) At 3000K, what is the minimum pressure needed before graphite changes into diamond? At the phase change, determine the degrees of freedom using Gibbs phase rule.

(b) What is the triple point temperature T_p for carbon? At the triple point, determine the degrees of freedom using Gibbs phase rule.

(c) Based on the phase diagram, are diamonds stable under normal conditions e.g. 1 atm and room temperature? If not, why are people able to wear diamonds without keeping them under high pressure?
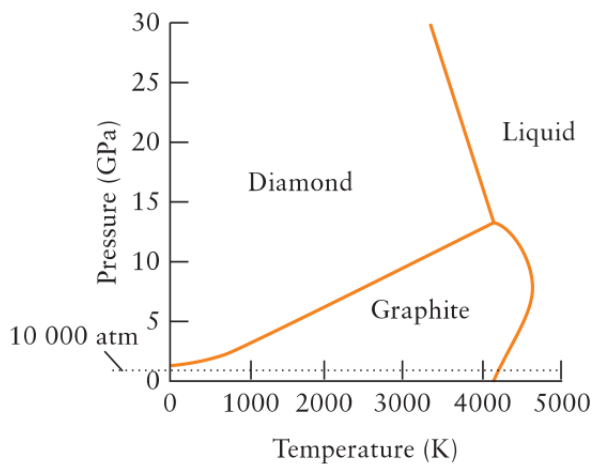

Figure 1: Phase diagram for carbon

2. (3 pts) **Vapor Pressure** Explain how the vapor pressure of a liquid is affected by each of the following changes in conditions:

(a) an increase in temperature

(b) a decrease in surface area of the liquid

(c) an increase in the surface tension

3. (4 pts) **Clausius–Clapeyron Equation** The Clausius–Clapeyron equation relates the vapor pressure and temperature of the system given by

$$P_f = P_i e^{-\frac{\Delta H^\circ_{\text{vap}}}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)} \tag{1}$$

where P is the vapor pressure, T is the temperature, and $\Delta H^\circ_{\text{vap}}$ is the enthalpy of vaporization. Report results to 3 significant figures.

(a) At standard atmospheric pressure, the vapor pressure of water at $80°C$ is 355.26 Torr. Determine the $\Delta H^\circ_{\text{vap}}$ for water. *Hint:* What is the vapor pressure of water at $100°C$?

(b) Using $\Delta H^\circ_{\text{vap}}$ in part (a), determine the amount of energy needed to heat 1 L of water from $10°C$ to $120°C$? Heat capcities of liquid water and water vapor are 4.184 J/(g $°C$) and 1.996 J/(g $°C$), respectively.

4. (7 pts) **Real Gases** The Van der Waals equation extends the ideal gas equation to include the effects of interaction between molecules of a gas given by

$$(P + \frac{a}{v^2})(v - b) = RT \tag{2}$$

where P is the pressure, v is the molar volume, T is the temperature, a and b are constants accounting for the non-ideality of the gas. Iron pyrite, FeS_2, is the form in which much of the sulfur exists in coal. In the combustion of coal, oxygen reacts with FeS_2 to produce iron(III) oxide and sulfur dioxide, which is a major source of air pollution and contributes to acid rain. The van der Waals parameters for SO_2 are $a = 6.865$ L^2 atm mol^{-2} and $b = 0.0568$ L mol^{-1}.

(a) Write a balanced equation for the burning of FeS_2 in air to produce iron(III) oxide and sulfur dioxide. Include states.

(b) For SO_2 confined in a 1.00 L vessel at 32°C, calculate the pressure of the gas by using the ideal gas law and the van der Waals equation for 0.100 mol to 1.100 mol SO_2 at 0.200 mol increments.

(c) Calculate the percentage deviation of the ideal value from the van der Waals equation at each point in part (b).

(d) If we consider gases to be ideal when the observed pressure differs by no more than 5% from the ideal value, at what pressure does SO_2 become a "real" gas?

5. (4 pts) **Phase Changes** *Extra Credit:* Let's interpret phase changes in terms of the thermodynamic functions. Consider the plot of the temperature dependence of the molar Gibbs free energy G_m of the three phases of a substance in Fig. 2.

(a) Indicate on the plot what is most favored phase for each section? At each intersection, what is this indicating?

(b) Explain in terms of molecular behavior why the G_m of each phase decreases with temperature.

(c) Explain in terms of molecular behavior why the G_m of the vapor phase decreases more rapidly with temperature than that of the solid or liquid phase.
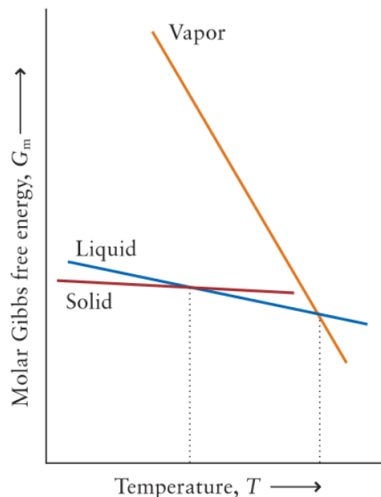

Figure 2: Gibbs free energy for three phases of a substance at a given pressure.

6. (10 pts) **Noncovalent Interactions** *Extra Extra Credit:* In lecture, Prof. Furche mentioned your TA Brian's Ph.D. work on noncovalent interactions (NIs). These include electrostatic, induction, and dispersion. The textbook description of dispersion is that these are instantaneous dipole moments and relatively "weak" compared to covalent bonds. However, this is not necessarily the correct interpretation. Attached is your TA Brian's *landmark* publication.

(a) Provide examples where NIs are important. Cite your sources.

(b) According to the paper, summarize the main results and conclusions.

(c) Given Fig. 3 taken from the paper, how should we physically interpret NIs?
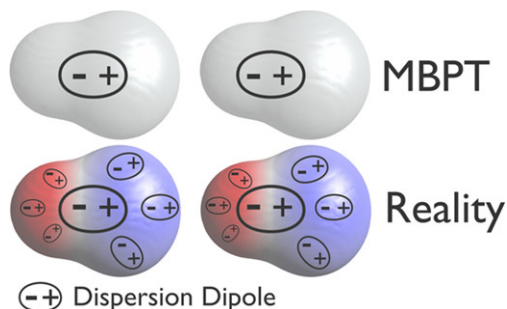

Figure 3: Illustration of dispersion interactions.

Partial credit may be given out. *Hint:* Attend Prof. Furche and Brian's office hours. **Due: March 15, 2022, at 11:59pm**

Optional Additional Problems: Ch. 11 - odd problems $35 - 45$, $53 - 89$