

# PHYS2020 Assignment 4

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5th of June 2020

## Question 1

(14 marks)

In this question you will introduce interactions and a cooling process into your Ideal Gas Matlab simulation from Assignment 2, in order to simulate phase changes (e.g. between solid, liquid and gas phase).

This question builds upon the interacting gas simulation you constructed in the previous assignment, examining how one can distinguish between different phases of matter within a system. The transitions between phases are typically identified through an “order parameter”, which is simply some sort of parameter which is selected because it has a different value for the order of the two phases. Generally, the order parameter changes rapidly during the transition from one phase to the other. For example, for a ferromagnetic material, the magnetisation is a natural order parameter – going from zero in the disordered phase where the temperature is sufficiently high as to randomise the orientation of each magnetic dipole, to non-zero when the thermal energy is insufficient to do this and the dipoles align.

- a. How many phases can you observe in your simulation of cooling of an interacting gas from Assignment 3? Describe them.

There appears to be at least two phases in the simulation from Assignment 3. The first of which represents a gaseous phase, where all of the particles are moving at varied velocities, in different directions, and appear to have little to no interaction with each other.

The other clearly observed phase would be closer to that of a liquid. In this phase, the particles seem to cluster in small to large groups, where they have similar velocities, move in approximately the same direction and keep a reasonably constant distance apart from each other.

On a reasonable timescale, a phase resembling that of a solid was not observed. In this state, large scale clusters with coherent movement and negligible relative velocity between particles were expected to be observed.

- b. Propose an order parameter that is able to distinguish between two of the phases and explain why you consider it a suitable choice.

A suitable order parameter could be the standard deviation of the acceleration as a result of intermolecular interactions. This parameter would describe the variation in the accelerations of the total particles, with a smaller value for the parameter implying that the particles are more highly ordered and resembles a denser state of matter. The most notable distinction between two phases would be that between liquid and gas, as liquid states imply weakly grouped and interacting particles while gaseous states imply no coherent groups or structures of particles at all.

- c. Calculate this order parameter for your simulation as a function of the temperature (probably the best approach here is to calculate the order parameter as a function of time while cooling the gas, and simultaneously calculate the temperature). Show that it varies abruptly as the phase transition is crossed, and use it to determine the transition temperature.

From assignment 3, the force acting upon a particle as a result of another could be calculated by

$$F = \frac{24\epsilon\sigma^6 (2\sigma^6 - r^6)}{r^{13}}$$

where  $\epsilon$  is the depth of the potential well,  $r$  is the distance between the two particles, and  $\sigma$  represents the range of the potential well. For a system of  $N$  particles, the total force acting upon one particle is

$$F = \sum_{i=1}^N \frac{24\epsilon\sigma^6 (2\sigma^6 - r_i^6)}{r_i^{13}}$$

and since  $a = F/m$ ,

$$a = \sum_{i=1}^N \frac{24\epsilon\sigma^6 (2\sigma^6 - r_i^6)}{mr_i^{13}}$$

and the average acceleration magnitude across all of the particles in the system is given by

$$\mu = \frac{1}{N} \sum_{\substack{i=1 \\ i \neq j}}^N \left| \frac{24\epsilon\sigma^6 (2\sigma^6 - r_{ij}^6)}{mr_{ij}^{13}} \right|$$

The order parameter is then

$$\begin{aligned} \sigma_a &= \sqrt{\frac{1}{N} \sum_{i=1}^N (|a_i| - \mu)^2} \\ &= \sqrt{\frac{1}{N} \sum \left( \left| \sum_{i=1}^N \frac{24\epsilon\sigma^6 (2\sigma^6 - r_i^6)}{mr_i^{13}} \right| - \frac{1}{N} \sum_{\substack{i=1 \\ i \neq j}}^N \left| \frac{24\epsilon\sigma^6 (2\sigma^6 - r_{ij}^6)}{mr_{ij}^{13}} \right| \right)^2} \end{aligned}$$

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- d. Explore your interacting particle model further in your own way. You could, for instance, explore how the phase transition temperature varies as you change the strength of the interactions; or you could add a different form of interaction to model new behaviour, for example, to model the flocking of birds or how ants collectively forage for food.

## Question 2

(14 Marks)

### Gibbs free energy of a van der Waals gas

The van der Waals equation of state is

$$P = \frac{NkT}{V - Nb} - \frac{aN^2}{V^2} \quad (1)$$

where the coefficients  $a$  and  $b$  account for attractive and repulsive interactions, respectively. The van der Waals equation predicts a critical point, below which a liquid-vapour mixture can form. The critical point appears as a point of inflexion on one of the isotherms.

a. Show that the critical point occurs at

$$V_c = 3Nb; \quad P_c = \frac{1}{27} \frac{a}{b^2}; \quad kT_c = \frac{8}{27} \frac{a}{b}$$

Firstly, the critical point occurs when both the derivative and double derivative of pressure with respect to volume is equal to zero. That is, the critical point occurs when  $\frac{\partial P}{\partial V} = \frac{\partial^2 P}{\partial V^2} = 0$ . The two derivatives are calculated as

$$\frac{\partial P}{\partial V} = \frac{2aN^2}{V^3} - \frac{NkT}{(V - Nb)^2} = 0 \quad (2)$$

$$\frac{\partial^2 P}{\partial V^2} = \frac{2NkT}{(V - Nb)^3} - \frac{6aN^2}{V^4} = 0 \quad (3)$$

Multiplying equation (2) by  $\frac{2}{(V - Nb)}$  gives

$$\frac{4aN^2}{V^3(V - Nb)} - \frac{2NkT}{(V - Nb)^3} = 0 \quad (4)$$

As both equations (3) and (4) are equal to 0, they may be added and solved to give

$$\begin{aligned} 0 &= \frac{2NkT}{(V - Nb)^3} - \frac{6aN^2}{V^4} + \frac{4aN^2}{V^3(V - Nb)} - \frac{2NkT}{(V - Nb)^3} \\ &= \frac{4aN^2}{V^3(V - Nb)} - \frac{6aN^2}{V^4} \\ &= \frac{2}{V^3(V - Nb)} - \frac{3}{V^4} \\ \frac{3}{V^4} &= \frac{2}{V^3(V - Nb)} \\ \frac{3}{V} &= \frac{2}{V - Nb} \\ \frac{V - Nb}{V} &= \frac{2}{3} \\ \frac{-Nb}{V} &= -\frac{1}{3} \\ V &= 3Nb \end{aligned}$$

Since this is at the critical point, denote  $V = V_c$ , and it has been shown that  $V_c = 3Nb$ . Using this

value, the critical temperature may be found by substituting  $V_c$  into equation (2):

$$\begin{aligned}
0 &= \frac{2aN^2}{(3Nb)^3} - \frac{NkT}{(3Nb - Nb)^2} \\
&= \frac{2aN^2}{27N^3b^3} - \frac{NkT}{4N^2b^2} \\
\frac{kT}{4Nb^2} &= \frac{2a}{27Nb^3} \\
kT &= \frac{8a}{27b}
\end{aligned}$$

Again, since this is at the critical point, denote  $kT = kT_c$ , and so it has been shown that  $kT_c = \frac{8}{27} \frac{a}{b}$ . Both of these critical volume and temperature values may be substituted into equation (1), yielding

$$\begin{aligned}
P &= \frac{N \frac{8a}{27b}}{3Nb - Nb} - \frac{aN^2}{(3Nb)^2} \\
&= \frac{8a}{2b \times 27b} - \frac{a}{9b^2} \\
&= \frac{8a}{54b^2} - \frac{6a}{54b^2} \\
&= \frac{a}{27b^2}
\end{aligned}$$

Finally, since this is at the critical point, denote  $P = P_c$ , and it has been shown that  $P_c = \frac{1}{27} \frac{a}{b^2}$ .

b. For numerical and plotting purposes, it is convenient to work with *reduced variables*:

$$t \equiv T/T_c; \quad p \equiv P/P_c; \quad v \equiv V/V_c$$

i.e. the critical point appears at  $(p, t) = (1, 1)$ . Show that the van der Waals equation in terms of reduced variables is:

$$p = \frac{8t}{3v - 1} - \frac{3}{v^2}$$

and the Gibbs free energy (from Eq 5.56 in Schroeder) is proportional to

$$g = -\frac{8}{3}t \ln(3v - 1) + \frac{8}{3} \frac{t}{3v - 1} - \frac{6}{v} + c(T)$$

where  $c(T)$  is some function of temperature that doesn't matter for our purposes.

Firstly, the van der Waals equation may be found in terms of reduced variables by dividing each side by  $P_c$

$$\begin{aligned}
\frac{P}{P_c} &= \frac{1}{P_c} \left( \frac{NkT}{V - Nb} - \frac{aN^2}{V^2} \right) \\
p &= \frac{27b^2 NkT}{a(V - Nb)} - \frac{27b^2 aN^2}{aV^2} \\
&= \frac{9bV_c kT}{a(V - Nb)} - \frac{3V_c}{V^2} \\
&= \frac{8V_c t}{3(V - \frac{1}{3V_c})} - \frac{3}{v^2} \\
&= \frac{8V_c t}{3V - V_c} - \frac{3}{v^2} \\
&= \frac{8t}{3v - 1} - \frac{3}{v^2}
\end{aligned}$$

Now, the Gibbs free energy as given by equation (5.56) in Schroeder may be found to be proportional to  $g$  by

$$\begin{aligned}
g &= -\frac{8}{3}t \ln(3v-1) + \frac{8}{3} \frac{t}{3v-1} - \frac{6}{v} + c(T) \\
&= -\frac{8}{3} \frac{T}{T_c} \ln\left(3\frac{V}{V_c} - 1\right) + \frac{8}{3} \frac{T}{T_c} \frac{1}{\left(3\frac{V}{V_c} - 1\right)} - \frac{6V_c}{V} + c(T) \\
&= -\frac{8}{3} \frac{27}{8} \frac{kTb}{a} \ln\left(\frac{V}{Nb} - 1\right) + \frac{8}{3} \frac{27}{8} \frac{kTb}{a \left(\frac{V}{Nb} - 1\right)} - \frac{18Nb}{V} + c(T) \\
&= -\frac{9kTb}{a} \ln\left(\frac{V-Nb}{Nb}\right) + \frac{9kTb}{a \left(\frac{V-Nb}{Nb}\right)} - \frac{18Nb}{V} + c(T) \\
&= \frac{9kTb}{a} \ln(Nb) - \frac{9kTb}{a} \ln(V-Nb) + \frac{9NkTb^2}{a(V-Nb)} - \frac{18Nb}{V} + c(T) \\
&= \frac{9kTb}{a} \ln(Nb) + \frac{9b}{aN} \left(-NkTb \ln(V-Nb) + \frac{N^2kTb}{V-Nb} - \frac{2aN^2}{V} + c(T)\right) \\
&= \frac{9b}{aN} (NkT \ln(Nb) + G)
\end{aligned}$$

And so  $G = \frac{aNg}{9b} - NkT \ln(Nb) \Rightarrow G \propto g$ .

- c. Working in terms of reduced variables, plot the van der Waals isotherm for  $t = 0.95$ . Perform the Maxwell constructions (either graphically or numerically) to obtain the vapour pressure.

The plotted isotherms for  $t = 0.95$  and  $t = 0.8$  can be seen in Figure 1

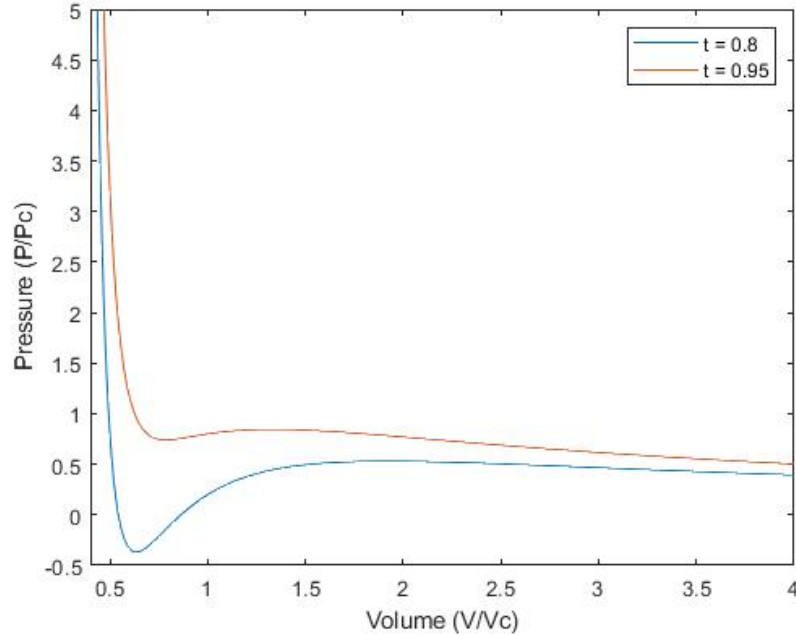


Figure 1: van der Waals Isotherms in Reduced Variables

By eyeballing Figure 1, the vapour pressure for  $t = 0.95$  looks to be at about  $P = 0.84P_c$ . This vapour pressure is the pressure of the point at which a horizontal straight line is drawn so as to enclose equal areas above and beneath the isotherm. For  $t = 0.8$ , the vapour pressure looks to be at about  $P = 0.3P_c$ .

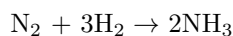
- d. Plot the Gibbs free energy (again in terms of reduced variables) for this same temperature as a function of pressure. Check that this predicts the same value for the vapour pressure as in part c.
- e. Repeat c. and d. for  $t = 0.8$ .

See respective sections.

### Question 3

(7 Marks)

Consider the production of ammonia from nitrogen and hydrogen,



at 298K and 1 bar. From the values of  $\Delta H$  and  $S$  tabulated at the back of this assignment, compute  $\Delta G$  of this reaction and check that it is consistent with value given in the table.

The change in Gibbs free energy of a system is given by

$$\Delta G = \Delta H - T\Delta S$$

For a reaction, this can be rewritten as

$$\begin{aligned}\Delta G_p &= G_{\text{products}} - G_{\text{reactants}} \\ &= (\Delta H_p - T\Delta S_p) - (\Delta H_r - T\Delta S_r)\end{aligned}$$

Where the subscripts  $p$  and  $r$  denote products and reactants respectively. Expressing the relationship in terms of the chemical variables given (and then substituting in the given values),

$$\begin{aligned}\Delta G_{2\text{NH}_3} &= (\Delta H_{2\text{NH}_3} - T\Delta S_{2\text{NH}_3}) - ((\Delta H_{\text{N}_2} + \Delta H_{3\text{H}_2}) - T(\Delta S_{\text{N}_2} + \Delta S_{3\text{H}_2})) \\ &= (2 \times -46.11 - 298 \times 2 \times 0.19245) - ((0 + 0) - 298(0.19161 + 3 \times 0.13066)) \text{ kJ} \\ &\approx -206.92 + 173.92 \text{ kJ} \\ &= -33 \text{ kJ}\end{aligned}$$

Since this reaction produces 2 molecules of ammonia, the calculated  $\Delta G$  should be twice as high as the tabulated value for  $\Delta G$  of one molecule of ammonia. As the table gives the value as  $\Delta G = -16.45 \text{ kJ} \Rightarrow 2\Delta G = -32.9 \text{ kJ}$ , this calculated value is approximately equal to the tabulated value ( $-33 \approx -32.9$ ).

## Question 4

(14 Marks)

This question considers the thermodynamics of the metal-superconductor phase transition. In general for a magnetic system the Gibbs free energy  $G$  can be written as a function of the temperature  $T$  and external magnetic field  $\mathcal{H}$ . The total magnetic field  $B$  is given by

$$B = \mu_0(\mathcal{H} + M)$$

where we assume all the vectors point in the same direction,  $M = m/V$  is the magnetisation per unit volume, and  $\mu_0$  is the permeability of free space. The thermodynamic identity for  $G$  in a magnetic system is

$$dG = -SdT - \mu_0 m d\mathcal{H}$$

where  $S$  is the entropy.

- Sketch the phase diagram of a type I superconductor as a function of temperature and external magnetic field.

The 'phase diagram' of a Type-I Superconductor with respect to external magnetic field and temperature can be seen in Figure 2

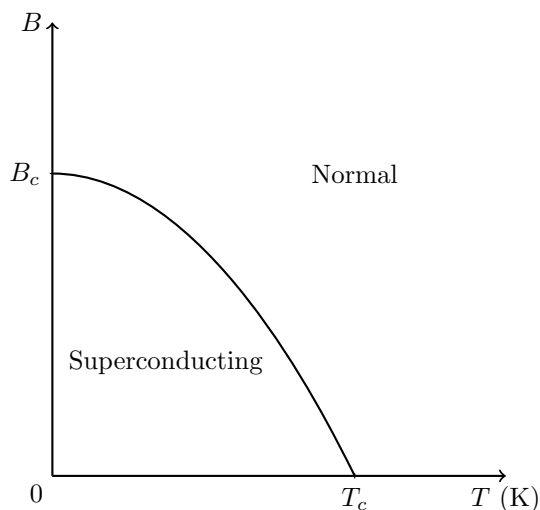


Figure 2: Phase Diagram of Type-I Superconductor ( $B$  vs  $T$ )

- Derive the Clausius-Clapeyron relation for the slope of the phase boundary:

$$\frac{d\mathcal{H}_c(T)}{dT} = -\frac{S_n - S_s}{\mu_0(m_n - m_s)}$$

where  $\mathcal{H}_c(T)$  is the external magnetic field at the phase boundary, and where the subscripts  $s$  and  $n$  denote values in the superconducting and normal metal phases, respectively.

At the phase boundary,  $dG_s = dG_n$ . So,

$$\begin{aligned}
-S_s dT - \mu_0 m_s d\mathcal{H}_c &= -S_n dT - \mu_0 m_n d\mathcal{H}_c \\
S_n dT - S_s dT &= \mu_0 m_s d\mathcal{H}_c - \mu_0 m_n d\mathcal{H}_c \\
(S_n - S_s) dT &= \mu_0 (m_s - m_n) d\mathcal{H}_c \\
\frac{d\mathcal{H}_c}{dT} &= \frac{(S_n - S_s)}{\mu_0 (m_s - m_n)} \\
&= -\frac{(S_n - S_s)}{\mu_0 (m_n - m_s)}
\end{aligned}$$

- c. The superconducting state displays perfect diamagnetism ( $B = 0$ ) due to the Meissner effect. The normal metal phase has a negligible magnetisation compared to the superconducting phase. Show that the latent heat per unit volume is given by

$$\ell = -\mu_0 T \mathcal{H}_c \frac{d\mathcal{H}_c}{dT}$$

Since  $B = 0$ ,  $\mathcal{H} = -M \Rightarrow \mathcal{H} = -m_s/V \Rightarrow V = -m_s/\mathcal{H}$ . We also have that the latent heat is  $L = T\Delta S$ , so  $\ell = L/V = T\Delta S/V$ . Utilising these, we can find the latent heat per unit volume in terms of  $\mathcal{H}$ :

$$\begin{aligned}
\ell &= \frac{T\Delta S}{V} \\
&= \frac{T(S_n - S_s)}{-m_s/\mathcal{H}_c} \\
&= -\frac{T(S_n - S_s)\mathcal{H}_c}{m_s}
\end{aligned}$$

Since  $m_s \gg m_n$ ,  $m_s \approx m_s - m_n$ . So,

$$\begin{aligned}
\ell &\approx -\frac{T(S_n - S_s)\mathcal{H}_c}{m_s - m_n} \\
&= T\mathcal{H}_c \frac{(S_n - S_s)}{m_n - m_s} \\
&= -\mu_0 T \mathcal{H}_c \frac{d\mathcal{H}_c}{dT}
\end{aligned}$$

- d. Show that when the transition occurs at zero field there is a discontinuity in the specific heat capacity (per unit volume) given by

$$c_s - c_n = -\mu_0 T_c \left( \frac{d\mathcal{H}_c}{dT} \right)^2$$



## Question 5

(14 Marks)

For this question make use of the attached table of thermodynamic data.

- a. Use the table of data to determine whether crystals of graphite or crystals of diamond are the thermodynamically stable form of carbon at room temperature and ambient pressure.

Since  $\Delta G$  is aimed to be minimised for a stable state of a substance, the crystalline structure of carbon with the lower  $\Delta G$  would be more stable at room temperature and pressure. The table of *Thermodynamic Properties of Selected Substances* gives  $\Delta_f G = 0\text{kJ}$  for graphite, and  $\Delta_f G = 2.9\text{kJ}$  for diamond, so graphite is the more stable structure at room temperature.

- b. Sketch the Gibbs free energy (at room temperature) of diamond and graphite as a function of pressure on the same graph. You may assume that the molar volumes do not vary significantly with pressure. Use your graph to estimate the pressure at room temperature at which the relative stability of diamond and graphite changes.

The sketch of Gibbs free energy vs Pressure may be seen in Figure 3

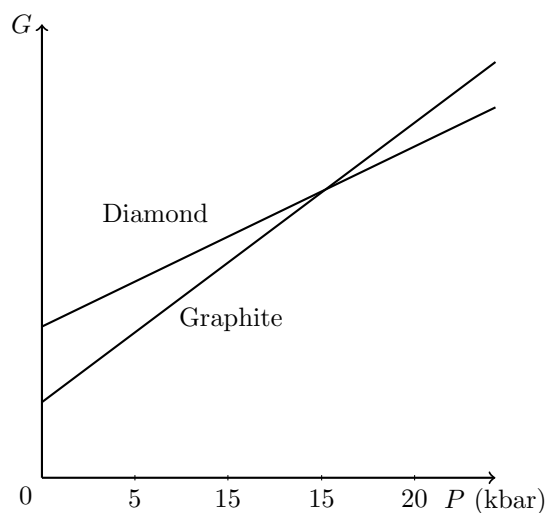


Figure 3: Gibbs Free Energy vs Pressure for Carbon Crystalline Structures

The point at which the relative stability of diamond vs graphite changes is the point at which their 'curves' intersect in Figure 3. By looking at the graph, this point appears to be at about 15 kbar of pressure.

- c. Estimate the slope  $\frac{dP}{dT}$  of the phase boundary between diamond and graphite at room temperature. Why should the slope of the phase boundary be zero near absolute zero temperature ( $T = 0\text{K}$ )?

The slope of the phase boundary,  $\frac{dP}{dT}$  is given by the Clausius-Clapeyron relation

$$\frac{dP}{dT} = \frac{S_g - S_d}{V_g - V_d}$$

where the subscripts  $g$  and  $d$  denote graphite and diamond respectively. Substituting in values from Appendix 1,

$$\begin{aligned} \frac{dP}{dT} &= \frac{5.74 - 2.38}{5.3 - 3.42} \text{ J}\cdot\text{K}^{-1}\cdot\text{cm}^{-3} \\ &= \frac{3.36}{1.88 \times 10^{-6}} \text{ J}\cdot\text{K}^{-1}\cdot\text{m}^{-3} \\ &\approx 1.79 \times 10^6 \text{ Pa} \cdot \text{K}^{-1} \\ &= 17.67 \text{ bar} \cdot \text{K}^{-1} \end{aligned}$$

At around absolute zero, the residual entropies of graphite and diamond approach each other, and so the numerator in the clausius-clapeyron relation approaches 0  $\Rightarrow \frac{dP}{dT} \rightarrow 0$ .

- d. Summarise your results in a sketch of the diamond-graphite phase diagram as a function of pressure and temperature. Explain why your diagram does not have a critical point.

The Diamond-Graphite Phase Diagram can be seen in Figure 4

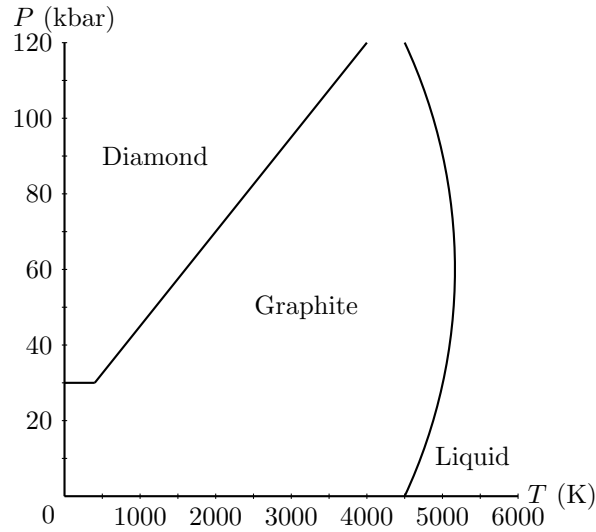


Figure 4: Diamond-Graphite Phase Diagram

By Schroeder, 'the stability region of the gas phase is not visible on this scale,' and so the liquid/gas critical point is not visible in Figure 4.

# Appendices

## Appendix 1: Thermodynamic Properties of Selected Substances

All of the values in this table are for one mole of material at 298 K and 1 bar. Following the chemical formula is the form of the substance, either solid (s), liquid (l), gas (g), or aqueous solution (aq). When there is more than one common solid form, the mineral name or crystal structure is indicated. Data for aqueous solutions are at a standard concentration of 1 mole per kilogram water. The enthalpy and Gibbs free energy of formation,  $\Delta_f H$  and  $\Delta_f G$ , represent the changes in  $H$  and  $G$  upon forming one mole of the material starting with elements in their most stable pure states (e.g., C (graphite), O<sub>2</sub> (g), etc.). To obtain the value of  $\Delta H$  or  $\Delta G$  for another reaction, subtract  $\Delta_f$  of the reactants from  $\Delta_f$  of the products. For ions in solution there is an ambiguity in dividing thermodynamic quantities between the positive and negative ions; by convention, H<sup>+</sup> is assigned the value zero and all others are chosen to be consistent with this value. Data from Atkins (1998), Lide (1994), and Anderson (1996). Please note that, while these data are sufficiently accurate and consistent for the examples and problems in this textbook, not all of the digits shown are necessarily significant; for research purposes you should always consult original literature to determine experimental uncertainties.

Substance (form)	$\Delta_f H$ (kJ)	$\Delta_f G$ (kJ)	$S$ (J/K)	$C_p$ (J/K)	$V$ (cm <sup>3</sup> )
Al (s)	0	0	28.33	24.35	9.99
Al <sub>2</sub> SiO <sub>5</sub> (kyanite)	-2594.29	-2443.88	83.81	121.71	44.09
Al <sub>2</sub> SiO <sub>5</sub> (andalusite)	-2590.27	-2442.66	93.22	122.72	51.53
Al <sub>2</sub> SiO <sub>5</sub> (sillimanite)	-2587.76	-2440.99	96.11	124.52	49.90
Ar (g)	0	0	154.84	20.79	
C (graphite)	0	0	5.74	8.53	5.30
C (diamond)	1.895	2.900	2.38	6.11	3.42
CH <sub>4</sub> (g)	-74.81	-50.72	186.26	35.31	
C <sub>2</sub> H <sub>6</sub> (g)	-84.68	-32.82	229.60	52.63	
C <sub>3</sub> H <sub>8</sub> (g)	-103.85	-23.49	269.91	73.5	
C <sub>2</sub> H <sub>5</sub> OH (l)	-277.69	-174.78	160.7	111.46	58.4
C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> (glucose)	-1273	-910	212	115	
CO (g)	-110.53	-137.17	197.67	29.14	
CO <sub>2</sub> (g)	-393.51	-394.36	213.74	37.11	
H <sub>2</sub> CO <sub>3</sub> (aq)	-699.65	-623.08	187.4		
HCO <sub>3</sub> <sup>-</sup> (aq)	-691.99	-586.77	91.2		
Ca <sup>2+</sup> (aq)	-542.83	-553.58	-53.1		
CaCO <sub>3</sub> (calcite)	-1206.9	-1128.8	92.9	81.88	36.93
CaCO <sub>3</sub> (aragonite)	-1207.1	-1127.8	88.7	81.25	34.15
CaCl <sub>2</sub> (s)	-795.8	-748.1	104.6	72.59	51.6
Cl <sub>2</sub> (g)	0	0	223.07	33.91	
Cl <sup>-</sup> (aq)	-167.16	-131.23	56.5	-136.4	17.3
Cu (s)	0	0	33.150	24.44	7.12
Fe (s)	0	0	27.28	25.10	7.11

Substance (form)	$\Delta_f H$ (kJ)	$\Delta_f G$ (kJ)	$S$ (J/K)	$C_P$ (J/K)	$V$ (cm <sup>3</sup> )
H <sub>2</sub> (g)	0	0	130.68	28.82	
H (g)	217.97	203.25	114.71	20.78	
H <sup>+</sup> (aq)	0	0	0	0	
H <sub>2</sub> O (l)	-285.83	-237.13	69.91	75.29	18.068
H <sub>2</sub> O (g)	-241.82	-228.57	188.83	33.58	
He (g)	0	0	126.15	20.79	
Hg (l)	0	0	76.02	27.98	14.81
N <sub>2</sub> (g)	0	0	191.61	29.12	
NH <sub>3</sub> (g)	-46.11	-16.45	192.45	35.06	
Na <sup>+</sup> (aq)	-240.12	-261.91	59.0	46.4	-1.2
NaCl (s)	-411.15	-384.14	72.13	50.50	27.01
NaAlSi <sub>3</sub> O <sub>8</sub> (albite)	-3935.1	-3711.5	207.40	205.10	100.07
NaAlSi <sub>2</sub> O <sub>6</sub> (jadeite)	-3030.9	-2852.1	133.5	160.0	60.40
Ne (g)	0	0	146.33	20.79	
O <sub>2</sub> (g)	0	0	205.14	29.38	
O <sub>2</sub> (aq)	-11.7	16.4	110.9		
OH <sup>-</sup> (aq)	-229.99	-157.24	-10.75	-148.5	
Pb (s)	0	0	64.81	26.44	18.3
PbO <sub>2</sub> (s)	-277.4	-217.33	68.6	64.64	
PbSO <sub>4</sub> (s)	-920.0	-813.0	148.5	103.2	
SO <sub>4</sub> <sup>2-</sup> (aq)	-909.27	-744.53	20.1	-293	
HSO <sub>4</sub> <sup>-</sup> (aq)	-887.34	-755.91	131.8	-84	
SiO <sub>2</sub> ( $\alpha$ quartz)	-910.94	-856.64	41.84	44.43	22.69
H <sub>4</sub> SiO <sub>4</sub> (aq)	-1449.36	-1307.67	215.13	468.98	