**Design Project**

Due date: 9 December 2013

You should work in a group of two people for this project. You should work together in such a way that the work is divided roughly evenly. I will ask you to provide a detailed list of the work each of you did on the project and the document must be signed by both of you.

Write a computer code in Matlab, C, C++, Java, or some other high-level language that does the following:

1. Use the Peng-Robinson EOS to compute $pVT$ properties of a fluid.

   \[ P = \frac{RT}{\tilde{V} - b} - \frac{ao(T, \omega)}{\tilde{V}^2 + 2b\tilde{V} - b^2} \]

   \[ \alpha(T, \omega)^{1/2} = 1 + (1 - T^{1/2}_r)(0.37464 + 1.5422\omega - 0.26992\omega^2) \]

2. Implement a cubic root solving algorithm to return the liquid and vapor roots (if applicable). Your code must prompt the user at the beginning of the run to determine if liquid or vapor properties are desired.

3. Compute the following molar departure functions: $\Delta \tilde{A}'$, $\Delta \tilde{H}'$, $\Delta \tilde{S}'$, $\Delta \tilde{G}'$, and the fugacity coefficient $\ln \phi$.

4. Implement a method for computing the ideal gas heat capacity and the ideal gas entropy from statistical mechanics. I.e., the program will read in the needed vibrational and rotational constants from a file, along with other needed information (number of atoms, linear or non-linear, etc.) and compute the ideal gas heat capacities and entropy as a function of temperature.

5. Implement a numerical integration method (Simpson’s rule, trapezoidal rule, Romberg integration, etc.) to compute integrals over heat capacity and entropy as needed. At very least your code should be able to compute the following:

   \[
   \int_{T_1}^{T_2} \tilde{C}'_V dT \\
   \int_{T_1}^{T_2} \frac{\tilde{C}'_V}{T} dT \\
   \int_{T_1}^{T_2} \tilde{S}' dT
   \]

6. The program must read the input data from a file.

7. The program must be easy for me to run! It should not require typing a good deal of information at the command line.

8. Turn in an electronic copy of the final program.
9. Test your program by computing $\Delta \tilde{A}$, $\Delta \tilde{G}$, $\Delta \tilde{S}$, and $\Delta \tilde{H}$, for NH$_3$ going from a liquid at $T_1 = 200$ K, $P_1 = 0.06$ bar to a vapor at $T_2 = 450$ K, $P_2 = 2.09$ bar.

My answers for this process are: $\Delta \tilde{A} = -45.73$ kJ/mol; $\Delta \tilde{G} = -42.00$ kJ/mol, $\Delta \tilde{S} = 129.5$ J/(mol K), and $\Delta \tilde{H} = 34.49$ kJ/mol. The liquid volume is $\tilde{V} = 2.647 \times 10^{-5}$ m$^3$/mol.

The liquid and vapor values of $\ln \phi$ are 0.33 and -0.005, respectively. If you want more information on this test case, please let me know.

10. Compute $\Delta \tilde{A}$, $\Delta \tilde{H}$, $\Delta \tilde{S}$, and $\Delta \tilde{G}$ for CH$_3$Cl for some $T_2$, $P_2$, $T_1$, $P_1$ of your choice, but with one of the state points is a liquid. Also report the values of $\ln \phi$ for each of the state points.

11. Provide a way for me to easily run your program for CH$_3$Cl at any state point of my choosing so that I may test your code for any arbitrary set of conditions. These points are for getting the correct answers. Your program must give the output in an easily readable form.

**Root finding algorithm for cubic EOS (See Numerical Recipes Ch. 5)**

A general cubic equation can be written in the form

$$x^3 + bx^2 + cx + d = 0$$

If the coefficients are REAL then the equation has at least one real root, and may have three real roots. If the coefficients are complex, then all three roots are complex.

For real coefficients compute the following quantities:

$$Q = \frac{b^2 - 3c}{9}$$
$$R = \frac{2b^3 - 9bc + 27d}{54}$$

If $Q^3 - R^2 \geq 0$ then the cubic equation has three real roots. Find the roots by computing

$$\theta = \arccos \left( \frac{R}{Q^{3/2}} \right)$$

Then the three roots are:

$$x_1 = -2Q^{1/2} \cos \left( \frac{\theta}{3} \right) - \frac{b}{3}$$
$$x_2 = -2Q^{1/2} \cos \left( \frac{\theta + 2\pi}{3} \right) - \frac{b}{3}$$
$$x_3 = -2Q^{1/2} \cos \left( \frac{\theta + 4\pi}{3} \right) - \frac{b}{3}$$

If $Q^3 - R^2 < 0$ there is only one real root given by

$$x_1 = -\text{sign}(R) \left\{ \left[ \left( R^2 - Q^3 \right)^{1/2} + |R| \right]^{1/3} + \frac{Q}{\left( R^2 - Q^3 \right)^{1/2} + |R|^{1/3}} \right\} - \frac{b}{3}$$

where $\text{sign}(R)$ is the sign of $R$, i.e., $\text{sign}(R) = 1$ if $R > 0$ and $\text{sign}(R) = -1$ if $R < 0$