Problem 1

Look at the dissociation of the halogen species F$_2$, Cl$_2$, Br$_2$, and I$_2$. For each, calculate the mole fraction of the atomic component at 500 K, 1000 K, 1500 K, and 2000 K at 1 atm. Use Burcat and/or NASA property fits. Repeat the calculation for H$_2$. Show your calculations and work. You can do this by hand calculation or spreadsheet calculation. If you do the latter approach, turn in your actual spreadsheet with the formulas. Does the ease of dissociation correlate with bond energy? Explain.

Problem 2

Hydrogen and iodine react to form HI at elevated temperatures. Estimate the equilibrium composition of a mixture of 1 mole of H$_2$ and 1 mole of I$_2$ at 1 and 0.1 atm at a temperature of 1100 K. Consider only I$_2$, I, H$_2$, and HI as possible species. Calculate values of $K_p$ from tabulated $c_p(T)$ or $h(T,P)$ & $s(T,P)$ data (list your sources). You may use a computational solver to get your advancements, but you must show all your equations. What species were neglected in this analysis? List as many as you can. Is neglecting these species a good approximation or not? Why or why not? (Hint: use the information from problem 1).

Problem 3

3) Estimate the heat of combustion for 1 mole of a) ethanol, b) propane, c) cyclopropane, d) propyne, e) 1,1,1-Propellane, f) bicyclobutane using first the bond energies, then tabulated values of heats of formation. Discuss any differences. For which types of molecules is the bond energy formulation most accurate? For which is it least accurate? What property of a molecule makes it less amenable to accurate energy calculation with tabular bond energies?