ME 501 Homework #1 Due Feb 3 2025 at 3 PM
Turn in Through Gradescope

(1)

Make a spreadsheet which takes constants from Chemkin format thermodynamic data and calculates c_p,u,h,s^o, and μ^o for ideal gas species. Use the “Burcat2023.xlxs” spreadsheet on the class website, from which you can cut and paste property constants for the desired species right into a spreadsheet. Your spreadsheet should look something like this:

	A	B	C	D	E	F	G	H	I	J
1	AR REF ELEMENT	g 5/97AR 1.	0. 0. 0.G	200.000 600	0.000 1000.			T_mid	(K)	1000
2	2.5000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00			R	Sets units	8.314
3	-7.4538E+02	4.3797E+00	2.5000E+00	0.0000E+00	0.0000E+00			T	(K)	500
4	0.0000E+00	0.0000E+00	-7.4538E+02	4.3797E+00	0.0000E+00			c_p	R units	20.785
5								h	RT units	4195.452
6								u	RT units	38.45225
7								s^o	R units	133.5503
8								μ^o	RT units	-62579.7
9										
10										
11	ALO	tpis96AL 1.O	1. 0. 0.G	200.000 600	0.000 1000.			T_mid	(K)	1000
12	2.8781E+00	1.9692E-03	-3.8630E-07	7.3179E-12	2.4845E-15			R	Sets units	1
13	7.2887E+03	9.5656E+00	3.3491E+00	-7.3081E-05	7.1016E-06			T	(K)	1400
14	-1.0614E-08	4.7071E-12	7.0573E+03	6.9746E+00	8.0966E+03			c_p	R units	4.907481
15								h	RT units	12904.28
16								u	RT units	11504.28
17								s^o	R units	32.80276
18								μ^o	RT units	-33019.6

Where the items in yellow are just pasted from the Burcat data, and you input values in the box in green, then the spreadsheet automatically calculates J4-J8. You can copy and paste rows 1-8 like I've done here multiple times to allow you to calculate multiple species on your spreadsheet. Keep this sheet for use in future class problems. Demonstrate your sheet by calculating c_p,u,h,s^o, and μ^o for the following species and conditions using Burcat constants: i) CO_2 at 2000 K. ii) HCN at 789 K, and iii) N_2H_4 at 900 K

(2)

Carbon sublimates at high temperature into gas products. Three of these are C, C_2, and C_3. At 5000 K and for pressures of 1 atm and 0.01 atm, find the gas composition of sublimated carbon assuming that only those three species exist. Use the approach that we used in class for the $CO/CO_2/O_2/O$ system (same computational approach, but different reactions), What other species could be considered in a more detailed analysis?

(3)

One mole of water vapor is maintained at 1 atm pressure. Initially, the system is at 300 K. A very short (effectively instantaneous) pulse of ultraviolet light dissociates 5% of the water molecules into OH and H molecules. There is no change in temperature or pressure during the light pulse. Assuming the final state of the system is pure H_2O vapor at 1 atm, what is the system temperature?

(4)

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?