

NORTH CAROLINA STATE UNIVERSITY

Department of Chemistry

Name _____

CH 431

Make up quiz

Physical Chemistry II

Due: April 30, 2003

- The Lennard-Jones of 6-12 potential is $u(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$. Determine the position of the minimum in the well r_{eq} in terms of σ by taking the derivative. Determine the well depth in units of ϵ at the value of r_{eq} by substitution of the minimum value into the expression for $u(r)$.
- Given that $\epsilon = 120k_B$ and $\sigma = 3.41 \text{ \AA}$ for argon estimate the van der Waal's a and b parameters for this gas using the derivation based on the second virial coefficient. Compare your calculated values of the van der Waal's a and b parameters to the tabulated values.
- A. Derive an expression for the Helmholtz energy A for argon treating it as a van der Waals gas. Use the system partition function for a van der Waals gas to obtain the result.
B. Calculate the minimum work required to compress argon from 1 atm to 200 atm of pressure assuming that it can be treated as a van der Waal's gas. Use the tabulated values for the van der Waal's parameters.
- Derive an expression for the isothermal compressibility and the expansion coefficient for argon treating it as a van der Waals gas. Calculate κ at 100 K and α 50 atm for argon treating it as a van der Waal's gas.
- Calculate the entropy change for the system, surroundings and the total entropy change for the isothermal expansion of an ideal gas from 1.5 L to 4.5 L against a constant external pressure of 3 atm.
- Calculate the thermodynamic efficiency of steam turbine operating at 370 K if the temperature at the outlet is 300 K.
- A. Given the following data at 50 °C determine the activity and activity coefficient for iodoethane (I) and ethylacetate (E) at a mole fraction of $x_E = 0.6282$.

x_I	P_I (torr)	P_E (torr)
0.0000	0.0	280.4
0.0579	20.0	266.1
0.1095	52.7	252.3
0.1918	87.7	231.4
0.2353	105.4	220.8

0.3718	155.4	187.9
0.5478	213.3	144.2
0.6349	239.1	122.9
0.8253	296.9	66.6
0.9093	322.5	38.2
1.0000	353.4	0.000

The Henry's law constants are $K_{H,I} = 345.3$ torr and $K_{H,E} = 421.2$ torr.

Henry's law standard state

$$a_I = \underline{\hspace{2cm}} \quad \gamma_I = \underline{\hspace{2cm}}$$

$$a_E = \underline{\hspace{2cm}} \quad \gamma_E = \underline{\hspace{2cm}}$$

Raoult's law standard state

$$a_I = \underline{\hspace{2cm}} \quad \gamma_I = \underline{\hspace{2cm}}$$

$$a_E = \underline{\hspace{2cm}} \quad \gamma_E = \underline{\hspace{2cm}}$$

Using the data above for 50 °C and a mole fraction $x_E = 0.6282$, calculate the free energy and entropy of mixing for a one mole of a regular solution of iodoethane and ethyl acetate using the Raoult's law standard state activity. Compare the ideal free energy of mixing with non-ideal free energy of mixing.

Ideal

$$\Delta_{\text{mix}} G = \underline{\hspace{2cm}}$$

$$\Delta_{\text{mix}} S = \underline{\hspace{2cm}}$$

Non-ideal

$$\Delta_{\text{mix}} G = \underline{\hspace{2cm}}$$

$$\Delta_{\text{mix}} S = \underline{\hspace{2cm}}$$