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ME 501

Exam #2
November 15, 2007
Prof. Lucht
ME 255

1. POINT DISTRIBUTION

Problem #1	**40 points**	____________________
Problem #2	**30 points**	____________________
Problem #3	**30 points**	____________________

2. EXAM INSTRUCTIONS

- Write your name on each sheet.
- This exam is closed book and closed notes.
- **Major hint: When calculating partition functions using the formula** $Z = \sum_j g_j \exp\left(-\varepsilon_j / k_B T\right)$**, write down the individual terms in the summation: you will need them later to calculate populations and properties.**
- Several equation sheets are attached.
- When working the problems, list all assumptions, and begin with the basic equations.
- If you do not have time to complete evaluation of integrals or of terms numerically, remember that the significant credit on each problem will be given for setting up the problem correctly and/or obtaining the correct analytical solution.

ME 501 Exam #2 11/15/2007 Name______________________________

1. **(40 points)** One (1.0) kmol of gaseous HF is contained in a rigid tank at pressure of 0.1 Pa at a temperature of 20 K (state 1). The temperature of the tank is raised to 30 K (state 2) by heat transfer. The pressure is low enough that the HF exhibits ideal gas behavior. Assume that the translational mode is fully excited at both the initial and final states.

(a) Assuming that HF is a rigid-rotator, calculate the internal energy change $U_2 - U_1$ (in J) for the constant volume heating process. Only the first four rotational levels (J = 0, 1, 2, 3) need to be considered for this problem; <u>explain why this is so</u>. **Do <u>not</u> assume that** $Z_{rot} = T / \theta_{rot}$**.** What is the rotational contribution to the internal energy change? Neglect the contributions of the vibrational, electronic, and nuclear modes.

Answer: 2.15x10^5 J

(b) Calculate the entropy change $S_2 - S_1$ (in J/K) for the gaseous HF. Use the same assumptions as in part (a). **Again, do <u>not</u> assume that** $Z_{rot} = T / \theta_{rot}$.

Answer: 8730 J/K

For HF: $\theta_{rot} = 30\ K\ ,\ m = 20\ \ amu$

ME 501 Exam #2 11/15/2007 Name____________________________

2. **(30 points)** A system has five energy levels with a constant energy level spacing:

$$\frac{\varepsilon_j}{k_B} = 100\, j \quad K \qquad\qquad j = 0, 1, 2, 3, 4$$

The degeneracy of each level increases with j and is given by $g_j = (j+1)^2 \times 10^{10}$.

(a) For an assembly of 10^7 particles, find the assembly energy E (in J) at a temperature of 50 K. Assume corrected-Maxwell-Boltzmann statistics. Note: this system does **not** have translational, rotational, etc. energy levels. It has only the energy levels specified.

Answer: 8.08x10^{-15} J

(b) For an assembly of 10^7 particles, find the assembly entropy S (in J/K) at a temperature of 50 K. Assume corrected-Maxwell-Boltzmann statistics.

Answer: 1.32x10^{-15} J/K

(c) Now consider an assembly of 8x10^{10} particles at absolute zero (0 K) that has the same five energy levels available. What is the assembly energy if the particles are Bose-Einstein particles (bosons)? What is the assembly energy if the particles are Fermi-Dirac particles (fermions)?

Answer: E_{BE}=0 J, E_{FD}=1.381x10^{-10} J

j	ε_j/k_B (K)	g_j
4	400	25×10^{10}
3	300	16×10^{10}
2	200	9×10^{10}
1	100	4×10^{10}
0	0	10^{10}

ME 501 Exam #2 11/15/2007 Name____________________________

3. **(30 points)** A rigid pressure vessel with a volume of 1 m^3 contains 0.10 kmols of the diatomic molecule WQ (a fictitious molecule) at 300K. The gas is heated to 2000 K. An absorption measurement of the W atom is performed and the after analyzing the results is concluded that $N_W = 5.12\text{x}10^{25}$.

(a) Is the experimental result $N_W = 5.12\text{x}10^{25}$ consistent with chemical equilibrium?

Answer: Yes

(b) What is the assembly pressure in Pascals (J/m^3)?

Answer: 3.07 MPa

Hint: Consider the reaction $WQ \leftrightarrow W + Q$. Also, remember that $P\forall = N k_B T$

Assume that diatomic species WQ is a rigid rotator and harmonic oscillator, neglect any ionization, and use the following characteristic temperature and dissociation energy data:

	θ_{rot}(K)	**θ_{vib}(K)**	**(D_0/k_B) (K)**
WQ	0.500	1500	10,000

The mass of monatomic species W is 80 amu and the mass of monatomic species Q is 4 amu. Consider the following electronic levels:

WQ: **Level 0:** $g_0 = 4$, $(\varepsilon_0 / k_B) = 0 \ K$

Level 1: $g_1 = 4$, $(\varepsilon_1 / k_B) = 400 \ K$

W: **Level 0:** $g_0 = 2$, $(\varepsilon_0 / k_B) = 0 \ K$

Q: **Level 0:** $g_0 = 4$, $(\varepsilon_0 / k_B) = 0 \ K$

Level 1: $g_1 = 8$, $(\varepsilon_1 / k_B) = 800 \ K$