國立中山大學102學年度碩士暨碩士專班招生考試試題

科目名稱：物理化學【材光系碩士班甲組】　　題號：439005

※本科目依簡章規定「可以」使用計算機（廠牌、功能不拘）　　

1. The density of water vapor at 327.6 atm and 776.4 K is 133.2 g/L. Determine the molar volume V_m of water and the compression factor Z from these data. In addition, calculate Z from the van der Waals equation with a = 5.464 L^2 atm/mol^2, and b = 0.03049 L/mol. Please comment the difference about these two data about Z. (15%)

2. A sample of 1.0 mol of perfect gas with C_v = 20.8 J/K is initially at 3.25 atm and 310 K. It undergoes reversible adiabatic expansion until its pressure reaches 2.50 atm. Calculate the final volume and temperature and the work done. (10%)

3. An ideal gas expands from initial volume from V_i to final volume V_f. Calculate the changes $\triangle U$, Q and W for the gas (in terms of n, T, V_i and V_f).
   (a) If the expansion is free expansion (5%)
   (b) If the expansion is adiabatic, and starts at temperature T_0. (5%)
   (c) If the expansion is isothermal at temperature T_0. (5%)

4. Consider a perfect gas contained in a cylinder and separated by a frictionless adiabatic piston into two sections A and B. All changes in B are isothermal; that is, a thermostat surrounds B to keep its temperature constant. There is 2.0 mol of the gas in each section. Initially $T_A = T_B$ = 300 K, $V_A = V_B$ = 2.0 L. Heat is added to Section A and the piston moves to the right reversibly until the final volume of Section B is 1.0 L. Calculate ΔS_A and ΔS_B. (10%)

5. The chemical shift of the CH_3 protons in acetaldehyde (ethanal) is δ = 2.20 and that of the CHO proton is 9.80. What is the difference in local magnetic field between the two regions of the molecule when the applied field is (a) 1.5 T, and (b) 15 T. (10%)

6. Sketch the form of an AMX NMR spectrum, where A, M, and X are protons with distinctly different chemical shift and $J_{AM} > J_{AX} > J_{MX}$. (10%)

7. Cotton consists of the polymer cellulose, which is a linear chain of glucose molecules. The chains are held together by hydrogen bonding. When a cotton shirt is ironed, it is first moistened, and then heated under pressure. Explain this process. (10%)

8. The diffusion coefficient of CCl_4 in heptanes at 25 °C is 3.17×10^{-9} m^2/s. Estimate the time required for a CCl_4 molecules to have a root mean square displacement of 5.0 mm. (10%)

9. Derive the rate law for the decomposition of ozone in the reaction $2O_3(g) \rightarrow 3O_2(g)$ on the basis of the following proposed mechanism:

$$(1)\ O_3 + M \underset{k_{-1}}{\overset{k_1}{\Leftrightarrow}} O_2 + O + M$$

$$(2)\ O_3 + O \xrightarrow{k_2} 2O_2$$

(10%)