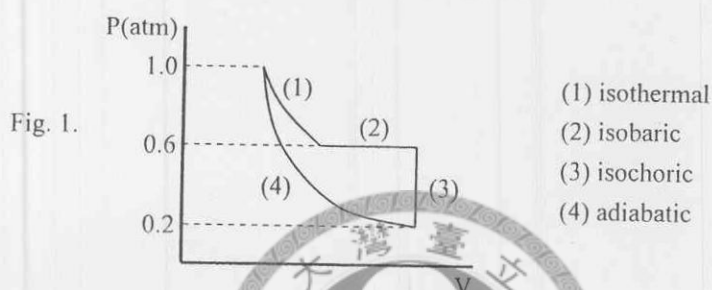


※注意：作答時，請於答案卷上標明作答之部分及其題號。

Part I 與 Part II 需分開作答

Part I:

1. One mole of an ideal gas ($C_v = 3R/2$), initially at 1.0 atm and 300 K, undergoes a reversible cycle containing four steps as shown in Fig. 1. 25%



Find ΔU , ΔS , and the work done for each step.

2. An electrochemical proton gradient is used to synthesize ATP in mitochondria. The pH inside the mitochondria membrane is 1.5 units lower than outside and the inside potential is -0.2 V relative to the outside. Inside the mitochondria, $[P_i] = [ADP] = [ATP] = 1$ mM. $T = 37^\circ\text{C}$. 15%

- (a) How much free energy is required to synthesize 1 mol of ATP inside the mitochondria (via the reaction: $\text{ADP} + P_i \rightarrow \text{ATP}$)? Assume that all the activity coefficients are 1. Is the process spontaneous?
(b) How much free energy is released by moving 1 mol of proton from the outside to the inside?
(c) If all the free energy from proton transport is used to synthesize ATP, how many protons have to be transported to synthesize 1 molecule of ATP?

3. A system has the following energy levels (ϵ_i) and degeneracies (g_i): 10%

ϵ_i/k	0	150 K	300 K	
g_i	1	2	3	
$\exp(-\epsilon_i/kT)$	1	0.606	0.368	at 300 K

Where, k is the Boltzmann constant.

- (a) Calculate the partition function of the system at 300 K.
(b) Calculate the fractional population of each energy level at 300 K.
(c) Calculate the entropy of the system at 300 K.

Part II

1. This problem concerns the molecular orbitals of benzene
 - (a) Write down the orbital energy levels for the π orbitals and fill with electrons
 - (b) Write down the molecular orbital for the lowest and the highest orbitals
 - (c) Explain the stability of benzene (12%)
2. The observed rate law for the reaction $2 \text{O}_3 \rightarrow 3 \text{O}_2$ is:
Rate = $k [\text{O}_3]^2 / [\text{O}_2]$. Propose a mechanism for the reaction. (11%)
3. Mathematical problems:
 - (a) Two fair dice (骰子) are rolled. What is the probability that at least one of them shows a "3"?
 - (b) Five coins are tossed. What is the probability that the number of heads(正) exceeds the number of tails(反)?
 - (c) Please integrate the function $f(x) = \exp(-3x)$ from 0 to infinity (12%)
4. Explain:
 - (a) SF_6 can be made but SCl_6 cannot
 - (b) The molecular orbital of Li_2
 - (c) Franck-Condon Principle (15%)