

科目：物理化學

適用：應化系

編號：374

考生注意：

1. 依次序作答，只要標明題號，不必抄題。
2. 答案必須寫在答案卷上，否則不予計分。
3. 限用藍、黑色筆作答；試題須隨卷繳回。

本 試 題

共 1 頁

第 1 頁

1. Explain the following terms (a) Chemical potential, (b) Second law of thermodynamics, (c) Space quantization, (d) Pauli exclusion principle, and (e) Boltzmann distribution. (20 %).
2. Calculate the changes in work, heat, internal energy, and entropy of the system, when 2 mol of argon at 300 K in a container of 0.5 dm^3 is allowed to expand to 1.0 dm^3 against a constant external pressure of 1.0 bar. (20 %) Hint: $\ln 2 = 0.69$
3. Derive the equation for the internal pressure of a gas $\pi_T = T \left(\frac{\partial p}{\partial T} \right)_V - p$ (10%)
4. Suppose that a molecular orbital has the (unnormalized) form $A + 2B$. Find a linear combination of the orbitals A and B that is orthogonal to this combination and determine the normalization constants of both combination using the overlap integral $S \left(\int AB d\tau \right) = 0.25$. (20%)
5. Write down the secular determinates for (a) linear H_3 and (b) cyclic H_3 , within the Huckel approximation. (10%)
6. Consider a second-order reaction of the type $A + 2B \rightarrow P$ carried out in a solution that was initially $0.060 \text{ mol dm}^{-3}$ in A and $0.030 \text{ mol dm}^{-3}$ in B. After 100 s, the concentration of B had fallen to $0.010 \text{ mol dm}^{-3}$. (a) Derive the integrated rate law of the product, and (b) calculate the rate constant. (20%)