

科目：物理化學 適用：應化所

編號：484

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. The lowest-frequency pure-rotational absorption line of $^{12}\text{C}^{32}\text{S}$ occurs at 48991.0 MHz. Find the bond distance in $^{12}\text{C}^{32}\text{S}$. (15%)
2. (a) If \hat{A} and \hat{B} are Hermitian operators, prove that their product $\hat{A}\hat{B}$ is Hermitian if only if \hat{A} and \hat{B} commute. (b) If \hat{A} and \hat{B} are Hermitian, prove that $\frac{1}{2}(\hat{A}\hat{B} + \hat{B}\hat{A})$ is Hermitian. (c) Is $\hat{x}\hat{p}_x$ Hermitian? (d) Is $\frac{1}{2}(\hat{x}\hat{p}_x + \hat{p}_x\hat{x})$ Hermitian? (20%)
3. (a) Please show the energy of free particle in a one-dimensional box of length l from the time-independent Schrödinger equation? (15%)
(b) A crude treatment of the π electrons of a conjugated molecule regards these electrons as moving in the free-particle-in-a-box potential. The Pauli exclusion principle allows no more than two electrons to occupy each box level. For butadiene, $\text{CH}_2=\text{CHCH}=\text{CH}_2$, take the box length as 7.0 \AA and use this model to estimate the wavelength (in nm) of the light absorbed when a π electron is excited from the highest-occupied to the lowest-vacant box level. The experimental value is 217 nm . (10%)
4. If $U = U(V, T)$ and $p = p(V, T)$ are functions of V and T and if $H = U + pV$, show that $\left(\frac{\partial H}{\partial T}\right)_p = \left(\frac{\partial U}{\partial T}\right)_V + p + \left(\frac{\partial U}{\partial V}\right)_T \left(\frac{\partial V}{\partial T}\right)_p$ (20%)
5. Calculate the entropy change when the argon at $25 \text{ }^\circ\text{C}$ and 1.00 bar in a container of volume 0.500 dm^3 is allowed to expand to 1.000 dm^3 and is simultaneously heated to $100 \text{ }^\circ\text{C}$. (20%)

Constants:

$$h = 6.626 \times 10^{-34} \text{ Js}$$