題號: 71

國立臺灣大學95學年度碩士班招生考試試題

科目:物理化學(A)

題號:71 共 1 頁之第 **全** 頁

Planck's constant	6.6×10^{-34} J s
Electron mass	9.1×10^{-31} Kg
Light speed	3.0×10^8 m/s
Typical C-C bond length	1.54 Å
Typical C=C bond length	1.34 Å

1. (30%) Suppose the volume of an ideal gas system expand reversibly and that there is no energy as heat flows into or out of the system during the expansion. Prove that the correct relation of the initial (P_1, V_1, T_1) and the final (P_2, V_2, T_2) states of the system is given by the following equation:

$$\left(\frac{T_2}{T_1}\right)^{C_V} = \left(\frac{V_1}{V_2}\right)$$

2. (40%) Consider the π electrons and the relevant molecular orbitals of butadiene molecule ONLY:



- (a) Draw the HOMO and LUMO orbitals. [10%]
- (b) The energy level of a particle in a one-dimensional box of length L is $E_n = \frac{n^2 h^2}{8mL^2}$ Based on the model of particle-in-a-box, estimate the longest wavelength for the electronic absorption spectrum of butadiene. [30%]
- 3. (30%) Explain the principles of nuclear magnetic resonance.