淡江大學 102 學年度碩士班招生考試試題

系別: 化學學系

科目:物理化學

考試日期:3月10日(星期日) 第2節

本試題共 五 大題, 二 頁

- 1)
- a) Please write down the time-dependent Schrodinger (TDS) equation for the particle system in 3-dimensional system. (5%)
- b) Please describe the physical meaning of each term within this TDS equation. (10%).
- 2)
- a) Based on the "particle in a box" quantum system please write down the time independent Schrodinger equation and their corresponding solutions of wavefunction and energy. (10%)
- b) Based on the solution of energy for the "particle in a box" quantum system please illustrate its application into the conjugate system of C=C-C=C in terms of the ability of electron donor and electron acceptor. (10%)
- c) Based on the solution of energy for the "particle in a box" quantum system please illustrate its application into the conjugate system of C=C-C=C in terms of its frequency to transform from its ground state into its first excited state. (10%)
- Zero law of thermodynamics states that if object A is in thermal equilibrium with object B, and object B is in thermal equilibrium with object C, then object C is also in thermal equilibrium with object A. This law allows us to build thermometers.
- a) Please briefly illustrate how the thermometer can be designed on the basis of zero law of thermodynamics. (10%)
- b) Based on your design of the thermometer please point out the requirements needed to have a very good thermometer. (10%)
- 4)

Consider an ideal gas system and a reversible change such that dQ = dU + PdV.

- a) Using U = 3nRT/2 and P=nRT/V, please prove that the dQ is not a state function. (10%)
- b) Now if we allow dQ to be divided through by T, then dQ/T = (3nR/2T) dT + (nR/V)dV. Please prove that dQ/T is a state function. (10%).
- Two of the simplest rate laws are given below in both their differential and integrated form.

Reaction	Order	Differential form	Integrated form
$A \rightarrow P$	zeroth	d[A]/dt = -k	$[\mathbf{A}] = [\mathbf{A}]_{0} - \mathbf{k}\mathbf{t}$
$A \rightarrow P$	first	d[A]/dt = -k[A]	$\ln[A] = \ln[A]_0 - kt$

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a) Please define what the half-life $t_{1/2}$ of a substance A is. (5%)

b) Please derive the equations for the half-lives for reactions of zeroth and first orders by substituting the values $t = t_{1/2}$ and [A] = 1/2 $[A]_0$ into the integrated rate laws as shown above. (10%)