※ 注意：請於答案卷上依序作答，並應註明作答之題號。

1. (10%) Draw Lewis electron dot diagrams for the following species:
(a) methane; (b) carbon dioxide;
(c) phosphorus trichloride; (d) perchlorate ion.

2. (15%) For describing a classical standing wave $\psi(x)$ in one dimension, it is
$$\frac{d^2\psi}{dx^2}+\frac{4\pi^2}{\lambda^2}\psi=0,$$
where λ is the wavelength of the standing wave. Show that this equation becomes a one-dimensional form of Schrödinger's wave equation
$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi,$$
when the de Broglie wavelength $\lambda=h/p$ for a particle moving in the presence of a potential, $V(x)$, is substituted into the classical equation and some algebraic rearrangement is made. (Hint: total energy is $E=p^2/2m+V(x)$)

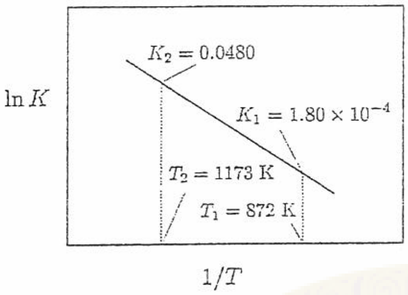
3. (15%)One of the main quantum laws relates the uncertainties of position Δx and momentum Δp of quantum particles. The uncertainty product cannot be less than a fixed value – a half of Planck's constant:
$$\Delta x\cdot\Delta p\geq\frac{\hbar}{2}$$
Without performing calculations arrange the following particles in the order of increasing minimal uncertainty of velocity, ΔV_{min}:
1) an electron in a H_2 molecule; 2) a H atom in a H_2 molecule; 3) a proton in the carbon nucleus; 4) a H_2 molecule within a nanotube; 5) a O_2 molecule in the room of 5 m width.

4. (15%) Sketch the molecular orbital energy diagrams of a linear chain consisted of one to four Li atoms and the associated orbitals, along with occupancies. Then generalize your results as to the number of nodes n in the middle and highest energy orbitals as a function of the number of atoms N.

5. (15%) Consider the isothermal expansion of 1.00mol of ideal gas at 27℃. The volume increases from 30.0L to 40.0L. Calculate q, w, ΔE, ΔH, and ΔS for two situations:
甲、a free expansion
乙、a reversible expansion

6. (15%) The following diagram shows the variation of the equilibrium constant with temperature for the reaction $I_2(g) \Leftrightarrow 2I(g)$. Calculate ΔG°, ΔH°, and ΔS° for the reaction at 872K.

見背面



7 (15%) Suppose we construct an electrochemical cell as shown in the following figure at the standard state ($Zn | Zn^{2+}(1M) \| Cl^-(1M) | AgCl | Ag$).

Assume that the extent of reaction is small enough to keep the concentrations essentially unchanged. During the discharge, heat will evolve from the resistor and from the cell, and we would measure the heat change by placing the cell and resistor in separate calorimeters. If we take Q_C as the heat change in the cell and Q_R as that in the resistor, we find $Q_C + Q_R = -233$ kJ/mol independent of R. In the limit of infinite R, Q_C approaches -43 kJ/mol and Q_R tends toward -190 kJ/mol.

a) What are the enthalpy, entropy and Gibbs energy changes of the reaction, $Zn + 2AgCl \rightarrow Zn^{2+} + 2Ag + 2Cl^-$.
b) What is the maximal thermodynamic efficiency (i.e. converting the heat released to non-PV work) of this electrochemical cell?

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