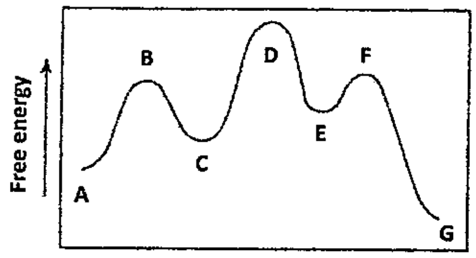
1. Given the following reaction coordinate diagram for the reaction of A to form G,




(A) How many intermediates are formed in the reaction? (3)
(B) The energy difference between which two steps is defined as activation energy? (3)
(C) What is the definition of "catalyst"? How a catalyst increase the rate of a reaction? (6)

2. The Haber-Bosch process is the main industrial procedure for producing ammonia. This procedure is generally conducted above 10 MPa with temperature around 500 °C with iron catalyst. The chemical equation is listed below:

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \quad \Delta H^\circ = -92.4 \text{ kJ/mol}$$

According to above description, please answer the following questions.
(A) What is the relationship between the rate of production of ammonia and the rate of consumption of hydrogen? (2)
(B) How lowering the pressure would affect the production of ammonia? (2)
(C) With the consistent volume, how adding helium gas would affect this equilibrium? (2)
(D) How lowering the temperature would affect this equilibrium? (2)
(E) Is this an endothermic or exothermic reaction? Why the Haber-Bosch process requires the temperature as 500 °C? (4)

3. Please explain following terms:
(A) The second law of thermodynamics (4)
(B) Entropy (4)
(C) Equilibrium constant (4)
(D) Buffer solution (4)

4. Please indicate a possible set of quantum numbers describing the electron in the following orbital or stage?
(A) $3s$ (3)
(B) $5d^6$ (3)
(C) $4p_x$ (3)

5. $\hat{H}\Psi = E\Psi$ is the simplest notation of the Schrödinger equation.

$$H = \frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)-\frac{Ze^2}{4\pi\varepsilon_0\sqrt{x^2+y^2+z^2}}$$

Considering the case of "particle in a box":

(A) Show that if $\Psi = A\sin rx + B\cos sx$ ($A$, $B$, $r$, and $s$ are constants) is a solution to the wave equation for the one-dimensional box, then (6)

$$r = s = \sqrt{2mE}\left(\frac{2\pi}{h}\right)$$

(B) Show that if $\Psi = A\sin rx$, the boundary conditions ($\Psi = 0$ when $x = 0$ and $x = a$) require that $r = \pm\frac{n\pi}{a}$, where n = any integer other than zero. (4)

(C) Show that if $r = \pm\frac{n\pi}{a}$, the energy levels of the particle are given by $E = \frac{n^2h^2}{8ma^2}$. (6)

(D) Show that substituting the value of $r$ given in into $\Psi = A\sin rx$ and applying the normalizing requirement gives $A = \sqrt{2/a}$. (5)

6. Considering a reaction with the general form as:

$$\mathrm{aA} \rightarrow \mathrm{bB}$$

At a certain temperature and $[\mathrm{A}]_0 = 1.00\times10^{-2}$ M, the data of concentration versus time were collected for this reaction, and a plot of ln[A] versus time resulted in a straight line with a slope value of $-3.00\times10^{-2}\,\mathrm{min}^{-1}$.

(A) Determine the rate law, the integrated rate law, and the value of the rate constant for this reaction. (8)

(B) Calculate the half-life for this reaction. (4)

(C) How much time is required for the concentration of A to decrease to $2.50\times10^{-3}$ M? (3)

7. You are given the rate constant as function of temperature for the exchange reaction

$$\mathrm{Mn(CO)_5(CH_3CN)^+ + NC_5H_5 \rightarrow Mn(CO)_5(NC_5H_5)^+ + CH_3CN}$$

| $T$(K) | k($\mathrm{min}^{-1}$) |
|---|---|
| 298 | 0.0409 |
| 305 | 0.0818 |
| 312 | 0.157 |

(A) Calculate $E_a$ from a plot of log k versus 1/$T$. (5)

(B) Estimate the value of k at 308 K. (5)

(C) What is the numerical value of the collision frequency factor, A, in the Arrhenius equation? (5)

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