

- (1) (12 %) Draw a qualitative plot of the following hydrogen atom wave function

$$\psi(r, \theta, \phi) = c_0 \sin \theta \sin \phi \left(\frac{6r}{a_0} - \frac{r^2}{a_0^2} \right) e^{-r/3a_0}$$

where c_0 is a constant and $a_0 = 0.53\text{\AA}$ is the Bohr radius. What are the principle quantum number n and the angular momentum quantum number l of this wave?

- (2) (12 %) Draw the MO energy diagrams for N_2 and O_2 . Note that the σ and π MOs have different ordering. What is the reason for this difference? What experiment(s) can detect the σ and π ordering?
- (3) (12 %) Write down the reaction for the methanol combustion. Use the following bond energies to estimate its ΔH° . Bond enthalpies O = O: 498 kJ mol^{-1} ; C - C: 348 kJ mol^{-1} ; C - H: 413 kJ mol^{-1} ; O - H: 463 kJ mol^{-1} ; C - O: 351 kJ mol^{-1} ; C = O: 728 kJ mol^{-1} .
- (4) (12 %) Given a reaction whose equilibrium constant K increases by a factor 1.0×10^5 when the temperature changes from 300K to 400K. Is ΔH° of this reaction positive or negative? Estimate the ΔH° by assuming that ΔS° and ΔH° do not change with the temperature.
- (5) (12 %) An acid has a $K_a = 1.0 \times 10^{-8}$. One adds $1.0 \times 10^{-5} \text{ mol}$ of this acid with water to form 1.0 L solution. Calculate the pH of this solution. ($K_w = 1.0 \times 10^{-14}$)
- (6) (10 %) An electron is confined in a 1D potential well where $0 \leq x \leq 1 \text{ nm}$. Given a matter wave function $\psi(x) = \sin(\pi x) + i \sin(2\pi x)$ where $i = \sqrt{-1}$. What is the probability distribution function of the electron? Make a plot of this probability function.
- (7) (10 %) Phenol has the $\text{p}K_a = 10$, which is much larger than the $\text{p}K_a = 16$ of alcohol. What is a explanation for the large difference?
- (8) (10 %) Draw a reasonable Lewis diagram for the compound PCl_5 (for example using valence shell expansion). Predict its molecular geometry.
- (9) (10 %) Across a thin cell membrane, the solution pH changes from 7.2 to 5.2. (a) Calculate the the electric potential difference across the membrane. (b) Which side (7.2 side or 5.2 side) has a higher potential?

Some physical constants: gas constant $R = 8.314 \text{ J mol}^{-1}\text{K}^{-1}$, elementary charge $e = 1.602 \times 10^{-19} \text{ C}$, Faraday constant $F = 96485 \text{ C mol}^{-1}$.

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