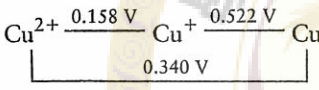


(I). 單選題 (選出一個最適當的答案): 每題 3 分. (答案直接填入“選擇題作答區”內)

- Which one of the following atoms has the highest electron affinity?  
(A) F (B) Cl (C) Br (D) I (E) At
- Which technique allows us to image and manipulate individual atoms?  
(A) X-ray diffraction (B) Nuclear magnetic resonance (C) Scanning tunneling microscopy (D) Transmission electron microscopy (E) All of the above
- The formal charge of the nitrogen atom in the nitrate ion is  
(A) -1 (B) 0 (C) +1 (D) +3 (E) +5
- The shape of SF<sub>4</sub> can be characterized as  
(A) Tetrahedron (B) Pyramid (C) Seesaw (D) Trigonal bipyramid (E) None of the above
- Considering proper number of significant figures,  $\frac{-36.334}{4.31} =$   
(A) 8.4 (B) 8.43 (C) 8.430 (D) 8.4302 (E) None of the above
- Which one of the following bonds is the most polar?  
(A) C-N (B) N-N (C) N-O (D) N-P (E) C-P
- What is the degeneracy of the first excited state of a particle in a three-dimensional cubic box?  
(A) 1 (B) 2 (C) 4 (D) 6 (E) None of the above
- The normalized wave function for a particle in a one-dimensional box is  $\psi_n(x) = \sqrt{2/L} \sin(n\pi x/L)$ , where  $L$  is the length of the box. What is the probability that the particle will lie between  $x = 0$  and  $x = L/4$  if the particle is in its first excited state?  
(A)  $\sqrt{2}/L$  (B)  $\frac{\sqrt{2L}}{2\pi}$  (C)  $\frac{\pi-2}{4\pi}$  (D)  $\frac{1}{4}$  (E) None of the above
- What is the number of radial nodes in a hydrogen 4f orbital?  
(A) 0 (B) 1 (C) 2 (D) 3 (E) None of the above
- A hydrogen 4f orbital has an angular momentum quantum number  $l = ?$   
(A) 0 (B) 1 (C) 2 (D) 3 (E) None of the above
- Koopman's theorem can be used to calculate which one of the following molecular properties?  
(A) Excitation energy (B) Ionization potential (C) Polarity (D) Electrostatic potential (E) None of the above
- Which one of the following diatomic molecules has the highest bond order?  
(A) C<sub>2</sub> (B) C<sub>2</sub><sup>+</sup> (C) O<sub>2</sub> (D) O<sub>2</sub><sup>+</sup> (E) F<sub>2</sub>
- Which one of the following  $\pi$ -conjugated molecule is aromatic?  
(A) Cyclopropenyl cation (B) Cyclopentadienyl cation (C) Ethylene (D) Hexatriene (E) None of the above
- What is the number of chiral centers in 4-ethyl-2,4-dimethylhexane?  
(A) 0 (B) 1 (C) 2 (D) 3 (E) 4
- The crystal field stabilization energy (CFSE) for a high-spin  $d^4$  ion in an octahedral complex is  
(A)  $-\frac{6}{5}\Delta_o$  (B)  $-\frac{3}{5}\Delta_o$  (C)  $-\frac{2}{5}\Delta_o$  (D) 0 (E) None of the above
- The van der Waals equation of state is  $\left(P + a\frac{n^2}{V^2}\right)(V - nb) = nRT$ . What is the coefficient  $a$  related to?  
(A) Strength of intermolecular interactions (B) Density of gas (C) Temperature (D) Excluded volume of the molecule (E) None of the above
- If 1.25 L of a carbonated beverage is bottled under a CO<sub>2</sub> pressure of 5.0 atm at 25°C, what is the number of moles of carbon dioxide dissolved in water? Use 1.00 g cm<sup>-3</sup> as the density of water and 1.65 × 10<sup>3</sup> atm as the Henry's law constant for carbon dioxide in water.  
(A) 0.21 (B) 0.42 (C) 0.17 (D) 0.34 (E) None of the above
- The order of the elementary reaction 2CH<sub>3</sub> → C<sub>2</sub>H<sub>6</sub> is ?  
(A) 0 (B) 1 (C) 2 (D) 3 (E) None of the above
- If 6.00 mol argon in a 100-L vessel initially at 300 K is compressed adiabatically until a temperature of 450 K is reached, what is the work done on the gas? (The gas constant R=8.314 JK<sup>-1</sup>mol<sup>-1</sup>).  
(A) 7.5 kJ (B) -7.5 kJ (C) 11.2 kJ (D) -11.2 kJ (E) None of the above

20. The enthalpy change for burning ketene ( $\text{CH}_2\text{CO}$ )  
 $\text{CH}_2\text{CO}(g) + 2 \text{O}_2(g) \longrightarrow 2 \text{CO}_2(g) + \text{H}_2\text{O}(g)$   
 is  $\Delta H_1 = -981.1 \text{ kJ}$  at  $25^\circ\text{C}$ . The enthalpy change for burning methane  
 $\text{CH}_4(g) + 2 \text{O}_2(g) \longrightarrow \text{CO}_2(g) + 2 \text{H}_2\text{O}(g)$   
 is  $\Delta H_2 = -802.3 \text{ kJ}$  at  $25^\circ\text{C}$ . What is the enthalpy change for the reaction below?  
 $2 \text{CH}_4(g) + 2 \text{O}_2(g) \longrightarrow \text{CH}_2\text{CO}(g) + 3 \text{H}_2\text{O}(g)$   
 (A)  $-178.8 \text{ kJ}$  (B)  $-623.5 \text{ kJ}$  (C)  $178.8 \text{ kJ}$  (D)  $623.5 \text{ kJ}$  (E) None of the above
21. At  $25^\circ\text{C}$ , the equilibrium constant for the reaction  
 $\text{N}_2(g) + \text{O}_2(g) \rightleftharpoons 2 \text{NO}(g)$   
 is  $4.2 \times 10^{-31}$ . Suppose a container is initially filled with nitrogen (0.41 atm), oxygen (0.59 atm), and nitrogen oxide (0.22 atm). What is the partial pressures of nitrogen after equilibrium is reached at  $25^\circ\text{C}$ ? ( $R=0.082 \text{ LatmK}^{-1}\text{mol}^{-1}$ ).  
 (A) 0.52 atm (B) 0.70 atm (C) 0.86 atm (D)  $3.9 \times 10^{-16} \text{ atm}$  (E) None of the above
22. The chemical formula of acetic acid is?  
 (A)  $\text{CHCOOH}$  (B)  $\text{HCOOH}$  (C)  $\text{CH}_3\text{CH}_2\text{OH}$  (D)  $\text{CH}_3\text{COOH}$  (E) None of the above
23. Suppose 1.000 mol of acetic acid is dissolved in enough water to give 1.000 L of solution. What is the pH of the solution? Acetic acid has a  $K_a$  of  $1.76 \times 10^{-5}$  at  $25^\circ\text{C}$ .  
 (A) 1.2 (B) 2.4 (C) 3.6 (D) 4.8 (E) None of the above
24. The reduction potential diagram of copper is  
  
 What is the standard voltage ( $\Delta\mathcal{E}^\circ$ ) for the disproportionation reaction of copper depicted below?  
 $2 \text{Cu}^+ \longrightarrow \text{Cu}^{2+} + \text{Cu}(s)$   
 (A) 0.340 V (B) 0.364 V (C) -0.340 V (D) -0.364 V (E) None of the above
25. What is the number of vibrational modes in the formaldehyde ( $\text{CH}_2\text{O}$ ) molecule?  
 (A) 3 (B) 6 (C) 9 (D) 12 (E) None of the above

(II). 敘述與計算題 (共 25 分):

26. Consider the molecular orbitals of a minimal basis set model for the hydrogen molecule ( $\text{H}_2$ ):  
 (26A) (5 marks) Give the MO correlation diagram for the neutral  $\text{H}_2$  molecule. Label each MO with its symmetry symbol ( $\sigma$ ,  $\pi$ , ...etc) and draw the MO graphically. Show the electronic configuration of the ground state of  $\text{H}_2$  in your MO diagram.  
 (26B) (3 marks) Give the electronic configurations and bond orders for the three molecules:  $\text{H}_2^+$ ,  $\text{H}_2$ ,  $\text{H}_2^-$ .  
 (26C) (2 marks) Give the many electron wave function of the ground state of  $\text{H}_2$ . Use  $\phi_{1s}^A$  and  $\phi_{1s}^B$  to represent the two basis functions.
27. (10 marks) Ethanol's enthalpy of vaporization is  $38.7 \text{ kJ mol}^{-1}$  at its normal boiling point,  $78^\circ\text{C}$ . Calculate  $q$ ,  $w$ ,  $\Delta U$ ,  $\Delta S_{\text{sys}}$ , and  $\Delta G$  when 1.00 mol ethanol is vaporized reversibly at  $78^\circ\text{C}$  and 1 atm. Assume that the vapor is an ideal gas and neglect the volume of liquid relative to that of the vapor. (The gas constant  $R=8.314 \text{ JK}^{-1}\text{mol}^{-1}$ ).
28. (5 marks) The reaction between nitric oxide and hydrogen,  
 $2\text{NO}(g) + \text{H}_2(g) \rightarrow \text{N}_2\text{O}(g) + \text{H}_2\text{O}(g)$   
 may proceed via the following mechanism:  
 $\text{NO}(g) + \text{NO}(g) \xrightleftharpoons[k_{-1}]{k_1} \text{N}_2\text{O}_2(g)$   
 $\text{N}_2\text{O}_2(g) + \text{H}_2(g) \xrightleftharpoons[k_{-2}]{k_2} \text{N}_2\text{O}(g) + \text{H}_2\text{O}(g)$   
 Give the rate law for the overall reaction using a steady-state approximation.