國立臺北科技大學102學年度碩士班招生考試

系所組別：3712 有機高分子研究所甲組

第二節　物理化學　試題（選考）

注意事項：

1. 本試題共十六題，配分共 100 分。
2. 請標明大題、子題編號作答，不必抄題。
3. 全部答案均須在答案卷之答案欄內作答，否則不予計分。

<<常用物理常數請參考最後一頁>>

第一部分、 單選題 ： 每題 3 分，共 30 分

1.Use the van der Waals equation for real gases to calculate the pressure exerted by 1.00 mole of ammonia at 27°C in a 750-mL container. (a = 4.17 L^2×atm/mol^2, b = 0.0371 L/mol)

(a) 23.2 atm
(b) 27.1 atm
(c) 32.8 atm
(d) 42.0 atm
(e) 32.8 torr

2.Select the gas with the largest root-mean-square molecular speed at 25°C.

(a) NH_3
(b) CO
(c) H_2
(d) SF_6
(e) All the gases have the same root-mean-square molecular speed at 25°C.

3.In the photoelectric effect, increasing the intensity of the light will

(a) ensure that electrons will be emitted from all metals.
(b) cause more electrons to be emitted from the metal if the frequency is sufficiently high.
(c) cause the electrons to be emitted with higher kinetic energy if the frequency is sufficiently high.
(d) have no effect on the experiment.
(e) both b and c

4.Which of the following sets of quantum numbers is allowed for an electron in a one electron atom?

(a) n=4, l=3, m=3, m_s=0
(b) n=3, l=1, m=2, m_s= –1/2
(c) n=2, l=0, m=1, m_s=1/2
(d) n=2, l=3, m=3, m_s=1/2
(e) n=6, l=5, m= –3, m_s= –1/2

5.According to the Bohr model of the atom, which is *highest* in energy?

(a) n=1 electron in He^+
(b) n=2 electron in H
(c) n=2 electron in He^+
(d) n=3 electron in Li^{2+}
(e) n=3 electron in H

6.Which of the following is true for a spontaneous process?

(a) $\Delta S_{univ} = 0$
(b) $\Delta S_{univ} < 0$
(c) $\Delta S_{univ} > 0$
(d) $\Delta S_{sys} = \Delta S_{surr}$
(e) none of the above

7.An increase in entropy for a closed system is always associated with

(a) an increase in the number of microstates available to the system.
(b) an increase in the number of molecules in the system.
(c) a and b
(d) None of the above

8.Consider the following quantities used in thermodynamics: E, H, q, w, S, G. How many of them are state functions?

(a) 0
(b) 1
(c) 2
(d) 3
(e) 4

注意：背面尚有試題

9.For the ground state term symbol, which of the following is correct?

(a) For H atom, it is $^1S_{1/2}$

(b) For F^{-1} atom, it is $^2S_0$

(c) For Sc atom, it is $^2S_0$

(d) For Ti atom, it is $^3F_2$

10.Which of the following molecules significantly absorb infrared radiation and therefore contribute to the "greenhouse effect"?

(a) N_2

(b) CO_2

(c) CH_4

(d) a and b

(e) b and c

(f) all of these above

第二部分、 非選擇題 :共 70 分　<< 請寫出計算或推導過程 >>

11.The average bond enthalpy of the O-H bond in water is defined as one-half of the enthalpy change for the reaction $H_2O(g) \rightarrow 2H(g) + O(g)$. The formation enthalpies, ΔH^0_f, for H(g) and O(g) are 218.0 and 249.2 $KJ\,mol^{-1}$, respectively, at 298.15K, and ΔH^0_f, for $H_2O(g)$ is -241.8 $KJ\,mol^{-1}$ at the same temperature.

(a)Use this information to determine the average bond enthalpy of the O-H bond in water at 298.15K. (5 分)

(b)Determine the average bond energy ΔU of the O-H bond in water at 298.15 K. Assume idea gas behavior. (5 分)

12.A key step in the production of sulfuric acid is the oxidation of $SO_2(g)$ to $SO_3(g)$:

$$2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$$

At 298 K, $\Delta G^0_{298} = -141.6\ KJ/mol$; $\Delta H^0_{298} = -198.4\ KJ/mol$; $\Delta S^0_{298} = -187.9\ J/K$

(a)Use these data to decide if this reaction is spontaneous at 25℃, and predict how ΔG will change with increasing temperature T. (3 分)

(b)Assuming that ΔH and ΔS are constant with T, is the reaction spontaneous at 900℃ (3 分)

(c)Calculate equilibrium constant K at 298 K. (4 分)

(d)If a sealed containers are filled with 0.500 atm of SO_2, 0.0100 atm of O_2, and 0.100 atm of SO_3, and kept at 298 K. In which direction, if any, will the reaction proceed to reach equilibrium? Please also calculate ΔG at this temperature. (10 分)

13.A study of the decomposition of 1 mole NO_2 to NO and O_2 gave out the following experimental rate constant data.

T (K)	$k\,(M^{-1}s^{-1})$
592	522
627	1700

Please calculate the activation energy Ea. (10 分)

14.Carbon-14 is a radioactive nucleus with a half-life of 5760 years. Living matter exchanges carbon with its surroundings (for example, through CO_2) so that a constant level of ^{14}C is maintained, corresponding to 15.3 decay events per minute. Once living matter has died, carbon contained in the matter is not exchanged with the surroundings, and the amount of ^{14}C that remains in the dead material decreases with time due to radioactive decay. Consider a piece of fossilized wood that demonstrates 2.4 ^{14}C decay events per minute. How old is the wood ? (10 分)

15.The strongest IR band of $^{12}C^{16}O$ occurs at $\tilde{\nu}$=2143 cm^{-1}. (a) Find the force constant of $^{12}C^{16}O$. (5 分) (b) Estimate the strongest IR band frequency of $^{13}C^{16}O$. (5 分)

16.Consider the molecule of hexatriene, CH_2=CH-CH=CH-CH=CH_2 . If we assume that the π electrons are free to move along the length of the molecule. Approximate the energy levels of this system by using a one-dimensional box model whose length is the summation of all lengths of C-C single bond and C=C double bond. Given the average C-C and C=C bond lengths are 1.54 Å and 1.34 Å, respectively.

(a)Please calculate the wavelength of light in the first transition of this molecule. (5 分)

(b)If the experimental wavelength of maximum absorption is λ_{max} = 268nm, please calculate the length of this molecule based on the experimental results. (5 分)

Physical constants:

Gas Constant : R = 0.0821 atm L/mol-K = 8.314 J /mol-K

Avogadro constant N_A = 6.022 x 10^{23} /mol

Electron charge : e = 1.602 x 10^{-19} C ; Electron rest mass : m_e= 9.109 x 10^{-31} kg

Neutron rest mass : m_n = 1.675 x 10^{-27} kg ; Proton rest mass : m_p = 1.673 x 10^{-27} kg

Planck's constant : h = 6.626 x 10^{-34} J・s ; Boltzmann's constant : k= 1.381x 10^{-23} J/K

Speed of light in a vacuum : c= 2.998 x 10^8 m/s

1 J = 1 kg m^2/s^2 = 1 C V ; 1 cal = 4.184 J ; 1 L-atm = 101.3 J;

1 atm = 1.01325×10^5 Pa ;　1Bar = 1×10^5 Pa