Chemistry I Midterm Exam

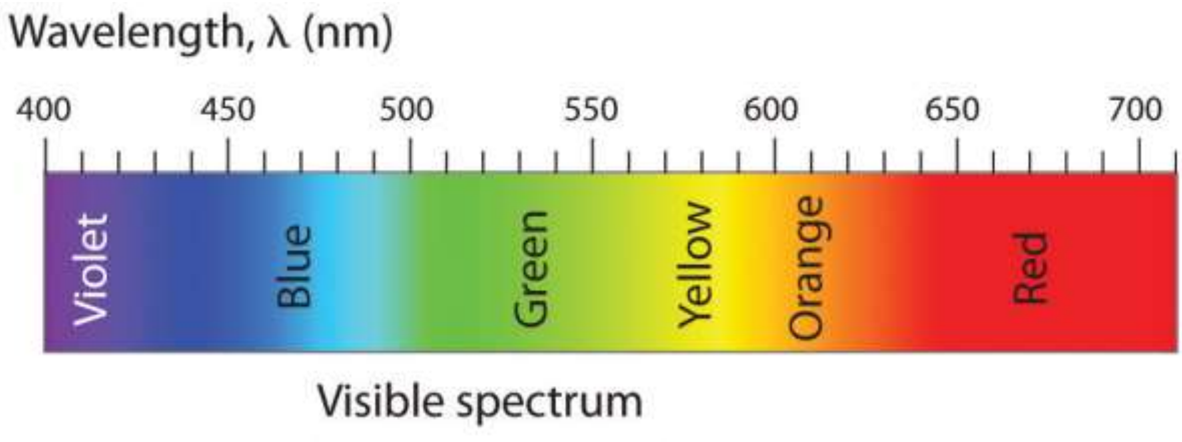
18:00-21:00, 13 November, 2015 (Total Score: 110 points)

1 1A	2 2A	3 3B	4 4B	5 5B	6 6B	7 7B	8 8B	9 8B	10 8B	11 1B	12 2B	13 3A	14 4A	15 5A	16 6A	17 7A	18 8A
1 H 1.008																	2 He 4.003
3 Li 6.941	4 Be 9.012											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.39	31 Ga 69.72	32 Ge 72.59	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.1	45 Rh 102.9	46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
55 Cs 132.9	56 Ba 137.3	57 *La 138.9	72 Hf 178.5	73 Ta 180.9	74 W 183.8	75 Re 186.2	76 Os 190.2	77 Ir 192.2	78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	89 †Ac (227)	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh (262)	108 Hs (265)	109 Mt (268)	110 Ds (271)	111 Rg (280)	112 Uub		114 Uuq		116 Uuh		118 Uuo

*Lanthanide series	58 Ce 140.1	59 Pr 140.9	60 Nd 144.2	61 Pm (147)	62 Sm 150.4	63 Eu 152.0	64 Gd 157.3	65 Tb 158.9	66 Dy 162.5	67 Ho 164.9	68 Er 167.3	69 Tm 168.9	70 Yb 173.0	71 Lu 175.0
†Actinide series	90 Th 232.0	91 Pa 231.0	92 U 238.0	93 Np 237.0	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (260)

1. Solve the following problems: (28%)
   (a) Derive a formula for the wavelength λ of a photon emitted in the $n_2 \rightarrow n_1$ transition in a one-electron atom with nuclear charge Z. (4%)
   (b) Prove that only four of the spectral lines in the emission spectrum of atomic hydrogen are located in the visible region of the electromagnetic spectrum. (Hint: consider only n_1 = 1 to 5) (8%)
   (c) Compute the wavelengths of the four spectral lines mentioned in the point (b) (4%)
   (d) Identify the color of the four spectral lines mentioned in the point (b) (4%)
   (e) How many spectral lines in the spectrum of the He^+ ion are located in the visible spectrum? Please prove your answer. (Hint: consider only n_1 = 1 to 5) (8%)

   You may need to know that the energy levels of a one-electron atom with nuclear charge Z are given by $E_n = -\frac{Z^2 h R_H}{n^2}$, where $R_H = 3.290\times10^{15}$ s^{-1} is the Rydberg constant and h = 6.626×10^{-34} J·s is the Planck constant. The relationship between the energy E of a photon and its frequency ν is given by $E = h\nu$ and the relationship between the wavelength λ of a photon and its frequency ν is given by λ = c/ ν. The speed of light is c = 2.999×10^8 $m\cdot s^{-1}$ and the visible region of the electromagnetic spectrum can be characterized by the following graph



2. The general solution of the 1D Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$

for the particle in a box with the potential

$$V(x)=\begin{cases}\infty & \text{for} \quad x<0\\ 0 & \text{for} \quad 0\le x\le L\\ \infty & \text{for} \quad x>L\end{cases}$$

is given by

$$\psi(x)=A\cos kx+B\sin kx$$

Application of the boundary conditions $\psi(0) = 0$ and $\psi(L) = 0$ gives a physically acceptable wave functions

$$\psi_n(x)=B\sin\left(n\pi\frac{x}{L}\right)$$

What is the form of physically acceptable wave functions when the potential is given by the following expression

$$V(x)=\begin{cases}\infty & \text{for} \quad x<0\\ 0 & \text{for} \quad 0\le x\le 3L\\ \infty & \text{for} \quad x>3L\end{cases}$$

(3%)

3. The orbital subshells with a definite value of the quantum number *l* are often designated with some letters. What are the letters for *l* = 0, 1, 2, 3, 4, 5? (6%)

4. Arrange the following atoms in order of decreasing atomic radius: K, Ne, Si, O and Mg.
(3%，順序錯誤一個扣一分，扣至 3 分)

5. Arrange the following atoms in order of increasing first ionization energy: N, He, Mg, O and Na. (3%，順序錯誤一個扣一分，扣至 3 分)

6. Write chemical equations corresponding to the following chemical concepts. Please write the correct state of the matters in the chemical equations.
   (a) The electron affinity of sulfur. (2%)
   (b) The third ionization energy of iron. (2%)
   Please write the correct state of the matter in the chemical equations.

7. The electron configurations of some excited atoms are listed below. Identify these atoms and write their ground-state electron configuration
   (a) $[Kr]\ 4d^7\ 5s^2\ 5p^5$ (3%)
   (b) $[Ne]\ 3s^1\ 3p^3\ 3d^1\ 4s^1$ (3%)
   (c) $[Xe]\ 4f^{12}\ 5d^8\ 6s^2\ 6p^3\ 6d^5$ (3%)

8. (a) Draw the Lewis structure for the CN^- ion and show formal charges. (3%) (b) In this picture, where do the lone pairs reside? (2%) (c) Sketch the molecular orbitals energy level diagram for the CN^-. (4%)

9. With the help of MO energy level diagrams, give the electron configurations for the ground state of He_2, HeH, and He_2^+. (3%) And determine their bond orders. (3%)

10. Compare the bond energy of F_2 with the energy change for the following process:

$$F_2(g) \rightarrow F^+(g) + F^-(g)$$

    What is the preferred dissociation for F_2, energetically speaking? Given (in kJ/mol): $D_0 = 154$, $E_{ea} = 328$, $I_1 = 1{,}680$. (5%)

11. With the help of MO energy level diagrams, give the electron configurations for the ground state of NO, O_2, and O_2^{2-}. Determine their bond order and indicate their magnetic properties. (9%)

12. Ketene, C_2H_2O does not have O-H bonds and is not cyclic.
    (a) Draw the Lewis structure of ketene. (2%)
    (b) Describe the hybridization states of the C atoms. (4%)
    (c) Draw the π-bonds of ketene. (4%)

13. Choose the correct answers from the list below for the molecules or ions in the table. (15%)

a. linear **b**. bent (angular) **c**. trigonal planar **d**. tetrahedral

e. trigonal bipyramidal **f**. octahedral **g**. trigonal pyramidal

h. distorted tetrahedron (seesaw) **i**. T-shaped **j**. square pyramidal

k. square planar **l**. *sp* **m**. sp^2 **n**. sp^3 **o**. sp^3d **p**. sp^3d^2 **q**. polar **r**. nonpolar

		Geometry	Hybridization of the central atom	polarity
1.	SO_3^{2-}			
2.	I_3^-			
3.	PCl_5			
4.	IF_5			
5.	H_2S			

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Answer

1.

(a) The transition from a level n_2 to a level n_1 ($n_2 > n_1$) is associated with an emission of a photon with energy $E = Z^2\, h\, R_H \left(\frac{1}{{n_1}^2} - \frac{1}{{n_2}^2}\right)$

The wavelength of this photon is given by $\lambda = \frac{hc}{E} = \frac{c}{Z^2 R_H} \frac{{n_2}^2 \cdot {n_1}^2}{{n_2}^2 - {n_1}^2}$ **(4%)**

($c/R_H = 0.912 \times 10^{-7}$ m = 91.2 nm)

(b) Since the visible part of the electromagnetic spectrum is located in the region between 400 and 700 nm, it is clear that the visible transitions $n_2 \to n_1$ must fulfill the following condition $400 \leq \frac{c}{Z^2 R_H} \frac{{n_2}^2 \cdot {n_1}^2}{{n_2}^2 - {n_1}^2} \leq 750$

For the series of transitions $n_2 \to N$, the transition with the largest wavelength is the transition N+1 $\to N$, for which

$$\lambda_{N,\,\max} = \frac{c}{Z^2 R_H} \frac{{n_2}^2 \cdot {n_1}^2}{{n_2}^2 - {n_1}^2}\bigg|_{n_1 = N, n_2 = N+1} = \frac{c\,(N+1)^2 \cdot N^2}{Z^2 R_H\,(2N+1)}$$

and the transition with the smallest wavelength is the transition ($n_2 = \infty$)$\to$N, for which

$$\lambda_{N,\,\min} = \frac{c}{Z^2 R_H} \frac{{n_2}^2 \cdot {n_1}^2}{{n_2}^2 - {n_1}^2}\bigg|_{n_1 = N, n_2 \to \infty} = \frac{c\,N^2}{Z^2 R_H}$$

These two expressions give the range $\left[\frac{c\,N^2}{Z^2 R_H}, \frac{c\,(N+1)^2 \cdot N^2}{Z^2 R_H\,(2N+1)}\right]$

of the wavelengths allowed for each series of transitions. In particular for hydrogen (Z = 1) for N = 1 to 5, we have:

Transitions to N = 1 (Lyman series): range [91.2-121.6 nm]

Transitions to N = 2 (Balmer series): range [364.8-656.6 nm]

Transitions to N = 3 (Paschen series): range [820.8-1876.1 nm]

Transitions to N = 4 (Bracket series): range [1459.2-4053.3 nm]

Transitions to N = 5 (Pfund series): range [2280.0-7461.8 nm]

It is clear that out of these 5 series, only the Balmer series is partially located in the visible region. The series with N > 5 are obviously out of the visible region.

More detailed calculations show that only 4 of spectral lines in the Balmer series are located in the visible spectrum:

$(n_2 = 3) \to (n_1 = 2)$ line with a wavelength $\lambda = 656\ nm$ (red)

$(n_2 = 4) \to (n_1 = 2)$ line with a wavelength $\lambda = 486.1\ nm$ (green, light blue)

$(n_2 = 5) \to (n_1 = 2)$ line with a wavelength $\lambda = 434.1\ nm$ (blue, dark blue)

$(n_2 = 6) \to (n_1 = 2)$ line with a wavelength $\lambda = 410.4\ nm$ (violet, indigo)

(8%)

(The next transition (n_2 = 7) ⟶ (n_1 = 2) in the Balmer series has a wavelength of 396.7 nm being just out of the visible region.)

(c) The wavelengths are: $656, 486, 434, 410\ nm$. For details, see above. **(4%)**

(d) The colors are: red, green, blue, and violet. For details, see above. **(4%)**

(e) For He^+, the ranges of the various spectral series are:

Transitions to N = 1 (Lyman series): range [22.8-30.4 nm]

Transitions to N = 2 (Balmer series): range [91.2-164.2 nm]

Transitions to N = 3 (Paschen series): range [205.2-469.0 nm]

Transitions to N = 4 (Bracket series): range [364.8-1013.3 nm]

Transitions to N = 5 (Pfund series): range [570-1865.4 nm]

It is clear that almost all spectral lines n_2 ⟶ (n_1 = 5) in the Pfund series (except for n_2 = 6 to 11) are located in the visible region of the electromagnetic spectrum. Since each of the series comprises of infinitely many spectral lines and only 6 of them is outside the visible region in the Pfund series for He^+, the correct answer is: For He^+, infinitely many spectral lines is located in the visible spectrum. **(8 %)**

2. $\psi_n(x) = B\sin\left(n\pi\frac{x}{3L}\right)$ **(3%)**

3. **(每個答案 1%，共 6%)**

$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$	$l = 5$
s	p	d	f	g	h

4. atomic radius: K > Mg > Si > O >Ne **(3%，順序錯誤一個扣一分，扣完為止)**

5. first ionization energy: Na < Mg < O < N < He **(3%，順序錯誤一個扣一分，扣完為止)**

6. (a) $S(g) + e^- \rightarrow S^-(g)$ **(2%)**

(b) $Fe^{2+}(g) \rightarrow Fe^{3+}(g) + e^-$ **(2%)**

7. (a) Sn **(1%)** ; $[Kr]\ 4d^{10}\ 5s^2\ 5p^2$ or $[Kr]\ 5s^2\ 4d^{10}\ 5p^2$ **(2%)**

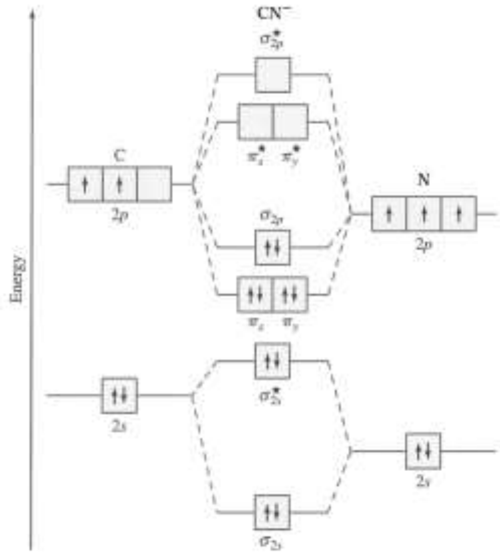
(b) S **(1%)** ; $[Ne]\ 3s^2\ 3p^4$ **(2%)**

(c) Po **(1%)** ; $[Xe]\ 4f^{14}\ 5d^{10}\ 6s^2\ 6p^4$ **(2%)**

8. (a) [:C≡N:]– ; formal charge: C = -1 , N = 0 **(3%)**

(b) The two lone pairs of electrons remain in the 2*s* (or *sp* hybridized) orbitals of C and N atom. **(2%)**

(c) **(4%)**



9. **(共 6%)**

	He_2	HeH	He_2^+	
electron configuration:	$\sigma_{1s}^2\ \sigma_{1s}^{*2}$	$\sigma_{1s}^2\ \sigma_{1s}^{*1}$	$\sigma_{1s}^2\ \sigma_{1s}^{*1}$	**(各 1%)**
bond order:	0	1/2	1/2	**(各 1%)**

10. The energy for the process $F_2(g) \rightarrow F^+(g) + F^-(g)$ can be found by adding the changes of energy for a series of steps that is equal to this process:

$F_2(g) \rightarrow F(g) + F(g)$	154 kJ/mol	
$F(g) \rightarrow F^+(g) + e^-$	1680 kJ/mol [I_1]	
$F(g) + e^- \rightarrow F^-(g)$	-328 kJ/mol [$-E_{ea}$]	
$F_2(g) \rightarrow F^+(g) + F^-(g)$	1506 kJ/mol	**(5%)**

11. NO : $\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \pi_{2py}^2\ \pi_{2pz}^2\ \sigma_{2px}^2\ \pi_{2py}^{*1}$ (or $\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \pi_{2p}^4\ \sigma_{2p}^2\ \pi_{2p}^{*1}$)

bond order = 2.5 ; paramagnetic

O_2 : $\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \sigma_{2px}^2\pi_{2py}^2\ \pi_{2pz}^2\pi_{2py}^{*1}\ \pi_{2pz}^{*1}$ (or $\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \sigma_{2p}^2\ \pi_{2p}^4\pi_{2p}^{*2}$)

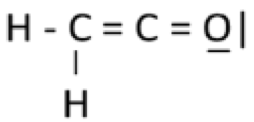
bond order = 2 ; paramagnetic

O_2^{2-} : $\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \sigma_{2px}^2\ \pi_{2py}^2\ \pi_{2pz}^2\ \pi_{2py}^{*2}\ \pi_{2pz}^{*2}$ (or $\sigma_{2s}^2\ \sigma_{2s}^{*2}\ \sigma_{2p}^2\ \pi_{2p}^4\pi_{2p}^{*4}$)

bond order = 1 ; diamagnetic

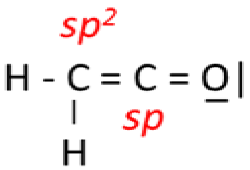
(每個答案個 1%，共 9%)

12. (a)



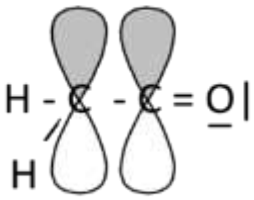
(2%)

(b)



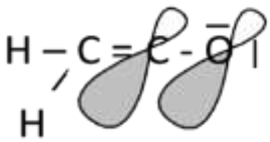
(二個碳原子各 2%，共 4%)

(c) C-C π bond: The p orbitals of the C atoms are perpendicular to the plane contains all atoms.



(2%)

C-O π bond: The p orbitals of the C and O atoms are in the plane contains all atoms.



(2%)

13. (每個答案 1%，共 15%)

		Geometry	Hybridization of the central atom	polarity
2.	SO_3^{2-}	**g**	**n**	**q**
2.	I_3^-	**a**	**o**	**r**
3.	PCl_5	**e**	**o**	**r**
4.	IF_5	**j**	**p**	**q**
5.	H_2S	**b**	**n**	**q**