

**2016 Fall Semester Midterm  
For General Chemistry I (CH101)**

**Date: October 22 (Sat), Time Limit: 19:00 ~ 22:00**

Student I.D. Number	Name

90 Normal Points + 8 Bonus Points

If you get 90 points out of 98 points, you will get the full 40% assigned to the mid-term exam. We suggest that you skim through all the problems quickly. There are some straightforward problems whose solution you can easily write down without much calculation.

### Your scores

- |               |                  |
|---------------|------------------|
| 1)            | out of 11        |
| 2)            | out of 6         |
| 3)            | out of 8         |
| 4)            | out of 6         |
| 5)            | out of 10        |
| 6)            | out of 10        |
| 7)            | out of 7         |
| 8)            | out of 14        |
| 9)            | out of 16        |
| 10)           | out of 10        |
| <b>Total:</b> | out of <b>98</b> |

You may refer to the following information.

hydrogen 1 H 1.0079																	helium 2 He 4.0026
lithium 3 Li 6.941	beryllium 4 Be 9.0122											boron 5 B 10.811	carbon 6 C 12.011	nitrogen 7 N 14.007	oxygen 8 O 15.999	fluorine 9 F 18.998	neon 10 Ne 20.180
sodium 11 Na 22.990	magnesium 12 Mg 24.305											aluminium 13 Al 26.982	silicon 14 Si 28.086	phosphorus 15 P 30.974	sulfur 16 S 32.065	chlorine 17 Cl 35.453	argon 18 Ar 39.948
potassium 19 K 39.098	calcium 20 Ca 40.078	scandium 21 Sc 44.956	titanium 22 Ti 47.867	vanadium 23 V 50.942	chromium 24 Cr 51.996	manganese 25 Mn 54.938	iron 26 Fe 55.845	cobalt 27 Co 58.933	nickel 28 Ni 58.693	copper 29 Cu 63.546	zinc 30 Zn 65.39	gallium 31 Ga 69.723	germanium 32 Ge 72.61	arsenic 33 As 74.922	selecnium 34 Se 78.96	bromine 35 Br 79.904	krypton 36 Kr 83.80
rubidium 37 Rb 85.468	strontium 38 Sr 87.62	yttrium 39 Y 88.906	zirconium 40 Zr 91.224	niobium 41 Nb 92.906	molybdenum 42 Mo 95.94	technetium 43 Tc [98]	ruthenium 44 Ru 101.07	rhodium 45 Rh 102.91	palladium 46 Pd 106.42	silver 47 Ag 107.87	cadmium 48 Cd 112.41	indium 49 In 114.82	tin 50 Sn 118.71	antimony 51 Sb 121.76	tellurium 52 Te 127.60	iodine 53 I 126.90	xenon 54 Xe 131.29
caesium 55 Cs 132.91	barium 56 Ba 137.33	57-70 * Lu 174.97	hafnium 72 Hf 178.49	tantalum 73 Ta 180.95	tungsten 74 W 183.84	rhenium 75 Re 186.21	osmium 76 Os 190.23	iridium 77 Ir 192.22	platinum 78 Pt 195.08	gold 79 Au 196.97	mercury 80 Hg 200.59	thallium 81 Tl 204.38	lead 82 Pb 207.2	bismuth 83 Bi 208.98	polonium 84 Po [209]	astatine 85 At [210]	radon 86 Rn [222]
francium 87 Fr [223]	radium 88 Ra [226]	89-102 * Lr [262]	rutherfordium 104 Rf [261]	dubnium 105 Db [262]	seaborgium 106 Sg [266]	bohrium 107 Bh [264]	hassium 108 Hs [269]	meitnerium 109 Mt [271]	unnilium 110 Uun [272]	ununium 111 Uuu [273]	ununium 112 Uub [277]	unununium 114 Uuq [289]					

$$\sin 2x = 2 \sin x \cos x$$

$$\cos 2x = \cos^2 x - \sin^2 x = 2 \cos^2 x - 1 = 1 - 2 \sin^2 x$$

$$\tan 2x = \frac{2 \tan x}{1 - \tan^2 x}$$

$$\frac{\tan^2 x - 1}{\tan x} = \frac{-2}{\tan 2x}$$

$$\cot 2x = \frac{\cot^2 x - 1}{2 \cot x}$$

$$\cos^2 x = \frac{1 + \cos 2x}{2}$$

$$\sin^2 x = \frac{1 - \cos 2x}{2}$$

$$\sin^3 x = \frac{3 \sin x - \sin 3x}{4}$$

$$\cos^3 x = \frac{3 \cos x - \cos 3x}{4}$$

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

$$E_n = -\frac{Z^2}{n^2} (\text{rydberg})$$

$$E = hv = h \frac{c}{\lambda}$$

$$\Delta x \Delta p > \frac{\hbar}{2\pi}$$

$$E(\lambda, T) = \frac{2hc^2}{\lambda^5} * \frac{1}{e^{\frac{hc}{\lambda kT}} - 1}$$

Planck constant(h) =  $6.626 \times 10^{-34}$  J·s

Elementary charge(e) =  $1.602 \times 10^{-19}$  C

Vacuum permittivity ( $\epsilon_0$ )=  $8.854 \times 10^{-12}$  J<sup>-1</sup>·C<sup>2</sup>m<sup>-1</sup>

Electron mass( $m_e$ ) =  $9.109 \times 10^{-31}$  kg

Speed of light in vacuum(c) =  $2.998 \times 10^8$  m/s

Rydberg constant =  $2.18 \times 10^{-18}$  J

$$\int d\tau = \int_0^\infty \int_0^\pi \int_0^{2\pi} r^2 dr \sin \theta d\theta d\phi$$

$$\int \sin^2 ax dx = \frac{x}{2} - \frac{1}{4a} \sin 2ax + C = \frac{x}{2} - \frac{1}{2a} \sin ax \cos ax + C$$

$$\int \sin^3 ax dx = \frac{\cos 3ax}{12a} - \frac{3 \cos ax}{4a} + C$$

$$\int x \sin^2 ax dx = \frac{x^2}{4} - \frac{x}{4a} \sin 2ax - \frac{1}{8a^2} \cos 2ax + C$$

$$\int x^2 \sin^2 ax dx = \frac{x^3}{6} - \left( \frac{x^2}{4a} - \frac{1}{8a^3} \right) \sin 2ax - \frac{x}{4a^2} \cos 2ax + C$$

$$r_n = -\frac{n^2}{Z} a_0, a_0 = 0.529 \text{ \AA}$$

$$E_n = \frac{h^2 n^2}{8ma^2}, n = 1, 2, \dots$$

$$E_n = \frac{-Z^2 e^4 m_e}{8\epsilon_0^2 n^2 h^2}, n = 1, 2, \dots$$

1. In ionic compounds, the potential energy ( $V(R_{12})$ ) is expressed as a function of the distance between the ions ( $R_{12}$ ), choosing as zero the potential energy of the neutral atoms when they are infinitely far apart. (Total 11 pts)

$$V(R_{12}) = A e^{-\alpha R_{12}} - B \left( \frac{(e)(-e)}{R_{12}} \right) + \Delta E_{\infty}$$

(1)                      (2)                      (3)

(a) What do the three terms of the equation ((1), (2), (3)) represent? (3 pts) (1 pt each, No partial pts)

Answer)

(1) : repulsion between the ions as they get very close together

(2) : attractive Coulomb potential

(3) : energy required to create the ions from their respective neutral atoms

1 pt each

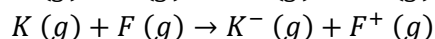
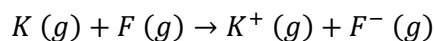
(b) Consider the ionic compound KF. Given that the first ionization energy of potassium is 419 kJ/mol and electron affinity of fluorine is 328 kJ/mol, calculate  $\Delta E_{\infty}$ . (1 pt) (No partial pts)

Answer)

$$\Delta E_{\infty} = IE_1(K) - EA(F) = +91 \text{ kJ mol}^{-1}$$

No partial points

(c) Calculate the energy changes ( $\Delta E$ ) for the following pairs of reactions:



Explain why  $K^+F^-$  forms in preference to  $K^-F^+$ .

The first ionization energy of fluorine is 1681 kJ/mol and the electron affinity of potassium is 48 kJ/mol. (2 pts) (0.5 pts for each reaction, 1 pt for correct explanation)

Answer)

1<sup>st</sup> reaction : 419-328=91 kJ/mol, 2<sup>nd</sup> reaction : 1681-48=1633 kJ/mol 0.5 pts each

1<sup>st</sup> reaction is energetically favored prior to form ionic compound. 1 pt

(d) Estimate the energy of dissociation ( $\Delta E_d$ ) to neutral atoms for KF, which has a bond length  $2.17 \times 10^{-10}$  m. (2 pts) (No partial pts)

Answer)

Example 3.6

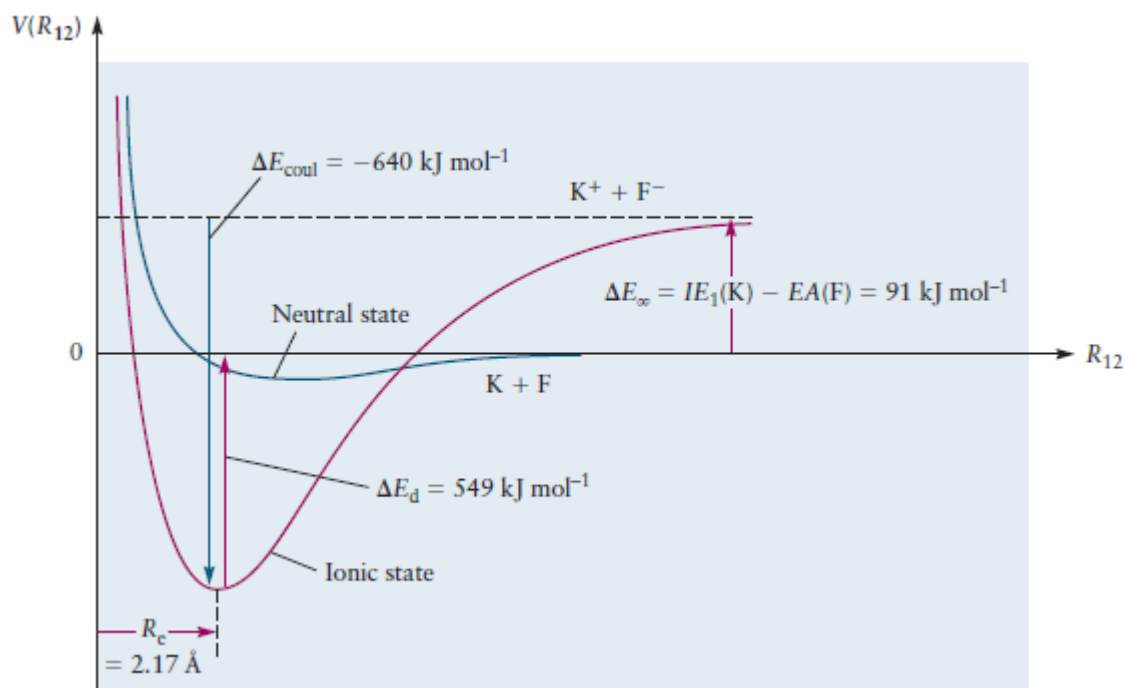
$$\begin{aligned}\Delta E_d &\approx -\frac{q_1 q_2}{4\pi\epsilon_0 R_c} \frac{N_A}{10^3} - \Delta E_\infty \\ &= -\frac{-(1.602 \times 10^{-19} \text{C})^2 (6.022 \times 10^{23} \text{mol}^{-1})}{(4)(3.1416)(8.854 \times 10^{-12} \text{C}^2 \text{J}^{-1} \text{m}^{-1})(2.17 \times 10^{-10} \text{m})(10^3 \text{J kJ}^{-1})} \\ &\quad -91 \text{ kJ mol}^{-1} \\ &= 640 \text{ kJ mol}^{-1} - 91 \text{ kJ mol}^{-1} \\ &= 549 \text{ kJ mol}^{-1}\end{aligned}$$

No partial points, pts are given if only the procedure and the answer are shown correctly.

(e) From the bond length and energy values calculated above, draw the potential energy curve of the ions  $K^+$  and  $F^-$  as a function of their internuclear separation  $R_{12}$ . (3 pts) (No partial pts)

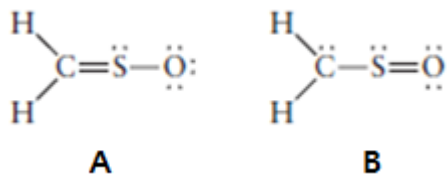
Answer)

Figure 3.13



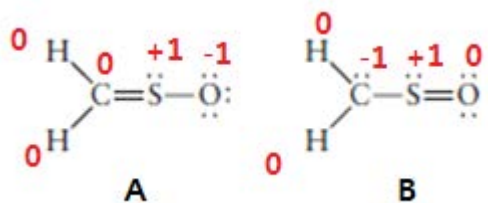
No partial points  $R_e$ ,  $\Delta E_d$ ,  $\Delta E_{\infty}$ , base line should be clearly shown.

2. Two possible Lewis structure are shown for sulfine ( $\text{H}_2\text{CSO}$ ). (Total 6 pts)



(a) Assign the formal charges on all atoms including 0 charge. (2 pts) (1 pt each, No partial pts)

Answer)



1 pt for each structure, pts are given if formal charges of all atom in structure are correctly shown.

(b) Of the two structures shown, which is “better”? Explain your selection. (2 pts) (No partial pts)

Answer)

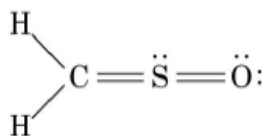
A : As negative formal charge is on the more electronegative element.

Keyword : negative formal charge/electronegative

Pts are given if the answer and explanation are correctly shown.

(c) Draw a best Lewis structure for sulfine, for which all atoms have a formal charge of zero. (2 pts)  
(No partial pts)

Answer)



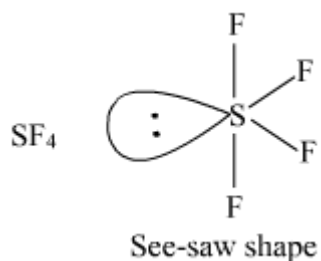
No partial points

3. Sketch the correct geometries of the following molecules, using the VSEPR method. The lone pairs must be shown and if the molecules have 3D structure, you must give exact 3D structure clearly.  
 (Total 8 pts, Each 2 pts) (-1 pt for lone pair missing)

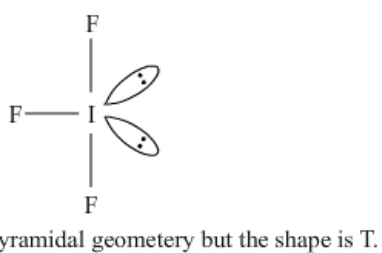
- (a) SF<sub>4</sub>
- (b) IF<sub>3</sub>
- (c) IF<sub>5</sub>
- (d) ICl<sub>3</sub> (Cl : chlorine)

Answer)

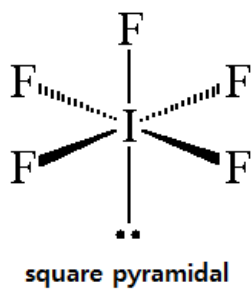
(a)



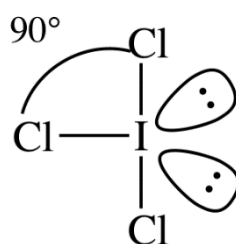
(b)



(c)



(d)



Minor mistakes(lone pair missing) -1 pts



4. Answer the following questions. (Total 6 pts)

(a) Explain the postulation used in the Bohr model. (2 pts) (No partial pts)

Answer)

The angular momentum of the electron is quantized in integral multiples of  $h/2\pi$ , where  $h$  is Planck's constant.

No partial points

(b) Calculate the energy required to remove the electrons from 1 mol of  $\text{Be}^{3+}$  in  $n = 4$  state. (2 pts) (-1 pt for calculation error)

Answer)

$$1.31 \times 10^6 \text{ J/mol}$$

$$E_n = -(2.18 \times 10^{-18}) \frac{Z^2}{n^2} \text{ J} = -(2.18 \times 10^{-18}) \text{ J}$$

The negative of the second answer is the input of energy needed to remove the electron from a single  $\text{Be}^{3+}$  ion in its  $n=4$  state. Multiply by Avogadro's number to put this on the basis of a mole of  $\text{Be}^{3+}$  ions

$$E = \frac{-(-2.18 \times 10^{-18} \text{ J})}{\text{atom}} \times \frac{6.022 \times 10^{23} \text{ atom}}{\text{mol}} = 1.31 \times 10^6 \text{ J/mol}$$

Calculation error -1 pt

(c) What frequency of light would be emitted in a transition from the  $n=4$  to the  $n=2$  state of this ion?  
(2 pts) (-1 pt for calculation error)

Answer)

$$9.87 \times 10^{17} \text{ s}^{-1}$$

The energy change in a  $\text{Be}^{3+}$  ion undergoing the  $4 \rightarrow 2$  transition equals the difference b/w the energies of the two states.

$$\Delta E = E_2 - E_4 = \left( -\frac{4^2}{2^2} \times 2.18 \times 10^{-18} \text{ J} \right) - \left( -\frac{4^2}{4^2} \times 2.18 \times 10^{-18} \text{ J} \right) = -6.54 \times 10^{-18} \text{ J}$$

The change in energy is negative because the  $\text{Be}^{3+}$  ion loses energy. It relaxes from the higher energy state to the lower. The energy gained by surrounding in the form of a photons in the  $4 \rightarrow 2$  transition is  $-6.54 \times 10^{-16} \text{ J}$ . Dividing by  $h$  gives the frequency of the photon,

$$\nu = -\frac{\Delta E}{h} = \frac{-(-6.54 \times 10^{-18} \text{ J})}{6.626 \times 10^{-34} \text{ Js}} = 9.87 \times 10^{15} \text{ s}^{-1}$$

Calculation error -1 pt

5. Answer the following questions. (Total 10 pts)

(a) A particle of mass  $m$  is placed in a 1D box with a length  $L$  ( $L > 0$ ). Inside the box the potential is zero, and outside it is infinite; therefore, the wavefunction goes smoothly to zero at both end of the box. Derive the normalized wave function ( $\psi_n$ ) and the energy ( $E_n$ ) for the one-dimensional particle-in-a-box. (6 pts) (Partial pts exist)

Answer)

Time independent Schrodinger Equation.

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x), \quad \hbar = \frac{h}{2\pi}$$

if  $0 < x < L, V(x) = 0$

$$\therefore -\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} = E\Psi(x) \quad \dots 1 \text{ pt}$$

$$\Psi(x) = A\sin(kx) + B\cos(kx) \quad \dots 1 \text{ pt}$$

By Boundary condition,  $\Psi(0) = 0, \Psi(L) = 0$

When  $x = 0, \sin(0) = 0$  and  $\cos(0) = 1$

Therefore  $B=0$  ( $\because \Psi(0) = B = 0$ )

$$\therefore \Psi(x) = A\sin(kx) \quad \dots 1 \text{ pt}$$

$$\Psi(L) = A \sin(kL) = 0$$

$$\therefore kL = n\pi \text{ where } n = 1, 2, 3 \dots$$

$$k = \frac{n\pi}{L} \dots 1 \text{ pt}$$

For normalization,

$$\int_0^L [\Psi(x)]^2 dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = A^2 \int_0^L \frac{1 - \cos\left(\frac{2n\pi x}{L}\right)}{2} dx = \frac{AL^2}{2} = 1$$

$$\therefore A = \sqrt{\frac{2}{L}}, \Psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \text{ where } n = 1, 2, 3 \dots \dots 1 \text{ pt}$$

$$\frac{d\Psi(x)}{dx} = kA \cos(kx)$$

$$\frac{d^2\Psi(x)}{dx^2} = -k^2 A \sin(kx) = -k^2 \Psi(x) = -\left(\frac{n\pi}{L}\right)^2 \Psi(x)$$

$$\text{Since } -\left(\frac{n\pi}{L}\right)^2 \Psi(x) = -\frac{2mE}{\hbar^2} \Psi(x), \quad -\left(\frac{n\pi}{L}\right)^2 = -\frac{2mE}{\hbar^2}$$

$$\therefore E = \frac{n^2 \hbar^2}{8mL^2} \text{ where } n = 1, 2, 3 \dots \dots 1 \text{ pt}$$

(b) A particle of mass  $m$  is placed in a 3D rectangular box with edge lengths  $2L$ ,  $L$ , and  $L$  ( $L > 0$ ). Inside the box the potential energy is zero, and outside it is infinite; therefore, the wavefunction goes smoothly to zero at the sides of the box. Calculate the lowest energy having degeneracy and give the quantum numbers of it for the particle in the box. (4 pts) (2 pts for energy calculation, 2 pts for quantum numbers)

Answer)

$$E_{n_x, n_y, n_z} = \frac{h^2}{8m} \left[ \frac{n_x^2}{(2L)^2} + \frac{n_y^2}{L^2} + \frac{n_z^2}{L^2} \right]$$

$$E_{112} = E_{121} = \frac{h^2}{8mL^2} \left( \frac{1}{4} + 4 + 1 \right) = \frac{21}{4} \frac{h^2}{8mL^2}$$

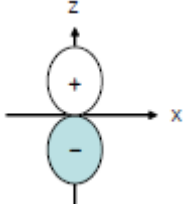
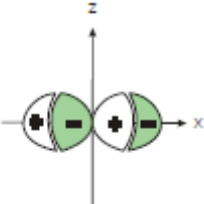
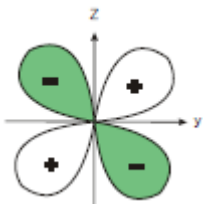
$$\text{energy: } E = \frac{21}{4} \frac{h^2}{8mL^2}$$

$$\text{quantum numbers: } (n_x, n_y, n_z) = (1, 1, 2), (1, 2, 1)$$

Energy : 2 pt

Quantum number : each 1 pt

6. There are several atomic orbitals below. Answer the following questions. (Total 10 pts)

(1)	(2)	(3)
		

(a) Write down the name of each of these orbitals. (3 pts) (1 pt each, No partial pts)

Answer)

(1)	(2)	(3)

(1) :  $2p_z$ , (2) :  $3p_x$ , (3) :  $3d_{yz}$

Each 1 pt

(b) For hydrogen atom (H), choose the two orbitals that have the same energy level. (2 pts) (No partial pts)

Answer)

(2), (3)

No partial points

(c) For boron atom (B), compare the energy level of (1), (2) and (3). (2 pts) (No partial pts)

Answer)

(1)<(2)<(3)

No partial points

(d) For one hydrogen atom (H), is light emitted or absorbed in an electron transition from the (3) to the (1) state? Calculate the frequency (in  $s^{-1}$ ) and wavelength (in nm) of light emitted or absorbed in this situation. (3 pts) (1 pt for emission/absorption, 1 pt for correct frequency, 1 pt for correct wavelength)

Answer)

Emission

$$\Delta E = -2.18 \times 10^{-18} \times \left(\frac{1^2}{2^2}\right) - \left(-2.18 \times 10^{-18}\right) \times \left(\frac{1^2}{3^2}\right)$$
$$= -3.03 \times 10^{-19} \text{ J}$$
$$3.03 \times 10^{-19} \text{ J} = h\nu \rightarrow \nu = \frac{3.03 \times 10^{-19}}{6.626 \times 10^{-34}} = 4.57 \times 10^{14} \text{ s}^{-1}$$
$$\lambda = \frac{c}{\nu} = \frac{2.998 \times 10^8}{4.57 \times 10^{14}} = 6.56 \times 10^{-7} \text{ m} = 656 \text{ nm}$$

Emission 1 pt, Frequency 1 pt, Wavelength 1 pt

7. Answer the following questions. (Total 7 pts)

(a) Chromium (Cr) is predicted by the building-up principle to have four unpaired electrons in its ground-state electron configuration, but in fact has six. Write the predicted and actual full ground-state electron configurations that explain this fact. You may use short hand noble gas configurations for core electrons. (2 pts) (1 pt for predicted electronic configuration, 1 pt for actual electronic configuration)

Answer)

Predicted electronic configuration :  $[\text{Ar}]3d^44s^2$

Actual electronic configuration :  $[\text{Ar}]3d^54s^1$

Each 1 pt

(b) Write the ground-state electron configuration of Sc and  $\text{Sc}^+$  ion, and predict them paramagnetic or diamagnetic. You may use short hand noble gas configurations for core electrons. (3 pts) (1 pt each for electron configuration, 0.5 pts each for paramagnetic or diamagnetic)

Answer)

Sc :  $[\text{Ar}]3d^14s^2$  (paramagnetic) 1 pt, 0.5 pt

$\text{Sc}^+$  ion :  $[\text{Ar}]3d^14s^1$  (paramagnetic) 1 pt, 0.5 pt



(c) Identify the element of period 2 that possesses the ionization energies (IE in  $\text{kJ mol}^{-1}$ ) in the table below. (2 pts)

1 <sup>st</sup> IE	2 <sup>nd</sup> IE	3 <sup>rd</sup> IE	4 <sup>th</sup> IE	5 <sup>th</sup> IE	6 <sup>th</sup> IE	7 <sup>th</sup> IE
1402.3	2856	4578.1	7475.0	9444.9	53266.6	64360

Answer)

N, Nitrogen

No partial points

8. Answer the following questions. (Total 14 pts)

(a) Construct the correlation diagram for  $O_2^-$ . (3 pts) (No partial pts)

Answer)

(b) Give the valence electron configuration for each of the following species:  $O_2^+$ ,  $O_2$ ,  $O_2^-$ ,  $O_2^{2-}$

(4 pts) (1 pt each)

Answer)

(c) Give the bond order of each species. (2 pts) (0.5 pts each)

Answer)

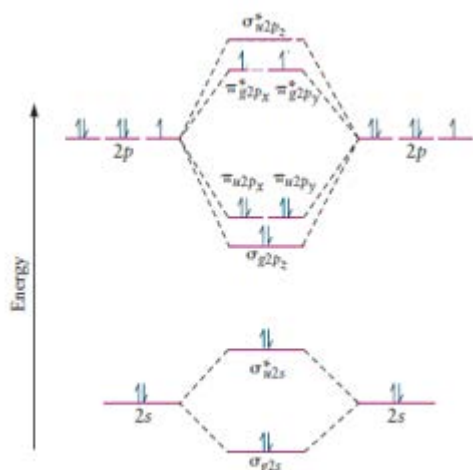
(d) Predict which species are paramagnetic. (3 pts) (No partial pts)

Answer)

(e) Predict the order of increasing bond dissociation energy among the species. (2 pts) (No partial pts)

Answer)

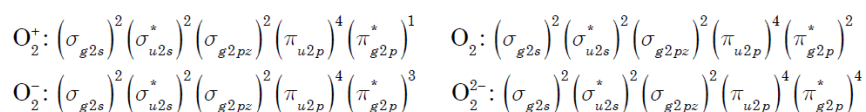
a)



From this diagram, there is one more electron in  $\pi_{g2px}^*$  or  $\pi_{g2py}^*$ .

a) The qualitative correlation diagram for  $O_2^-$  is identical to the diagram given for  $F_2$  in text Figure 6.17b except that an electron is removed from either the  $\pi_{2px}^*$  or the  $\pi_{2py}^*$  level.

b) The ground-state electron configuration of  $O_2$  is listed in Table 6.3. Derive the configurations of the ions in the problem by removal of electrons from the highest occupied or addition to the lowest unoccupied molecular orbitals:



c) The bond orders of the species are  $\frac{5}{2}$  (for  $O_2^+$ ), 2 (for  $O_2$ ),  $\frac{3}{2}$  (for  $O_2^-$ ) and 1 (for  $O_2^{2-}$ ).

b) All of the species except  $O_2^{2-}$  should be paramagnetic. A species with an odd number of electrons is automatically paramagnetic. The reason for the paramagnetism of ordinary  $O_2$  is discussed in the text.

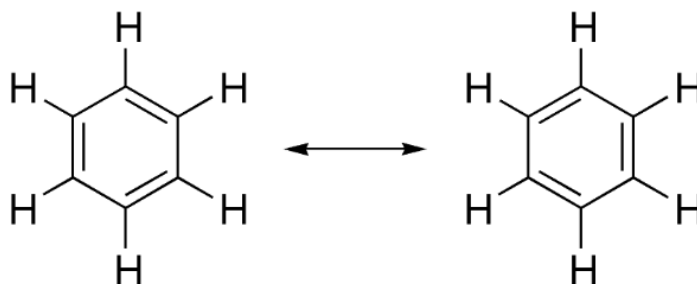
c) Members of the series  $O_2^+$  through  $O_2^{2-}$  are differentiated by successive addition of an electron. Each electron goes into a  $\pi^*$  antibonding orbital. The bond dissociation energy decreases along the series.

a, d, e) No partial points

9. Consider a benzene ( $C_6H_6$ ) molecule, having six-membered cyclic structure. (Total 16 pts)

(a) Based on the experimental observations that all C-C bonds are identical, draw the resonance hybrid Lewis diagrams for benzene. (2 pts) (No partial pts)

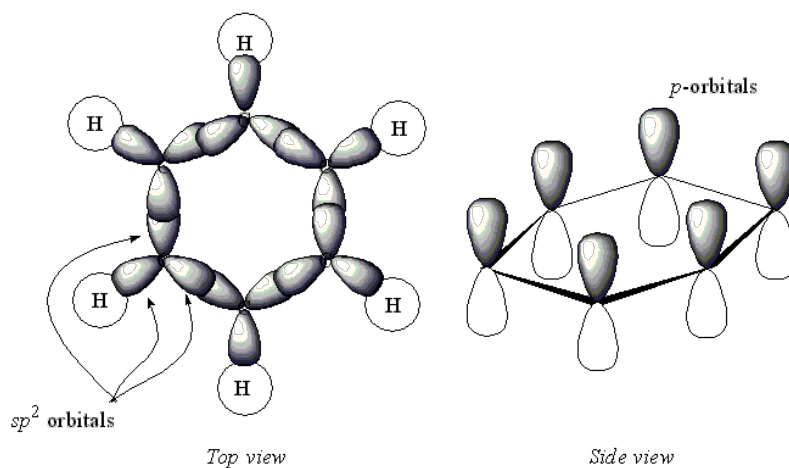
Answer)



No partial pts

(b) The structure of benzene can be explained using hybrid orbitals as well as Lewis diagrams. Draw 3D structure of benzene with hybrid orbitals, and mark for every bond if it is  $\sigma$  or  $\pi$  bond. (3 pts) (1 pt for correct 3D structure with hybrid orbitals, 1 pt for all  $\sigma$  bond marked, 1 pt for all  $\pi$  bond marked)

Answer)



Correct hybridization ( $sp^2$ ) 1 pt, sigma bond 1 pt, pi bond 1 pt

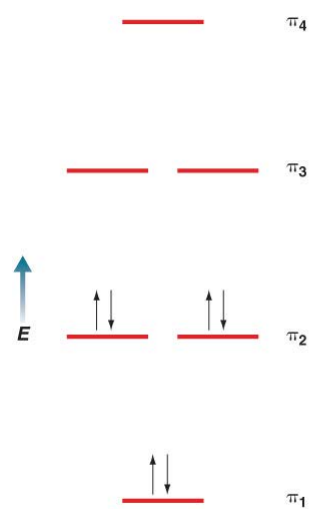
(c) As expected from (b), benzene molecule has delocalized  $\pi$  bonding. Draw molecular orbital energy level diagram for the  $\pi$  orbitals of benzene with its ground state electron configuration. (Hint : There are 6 p orbitals that can form delocalized  $\pi$  bonding) (3 pts) (2 pts for correct MO energy level diagram, 1 pt for correct electron configuration)

Answer)

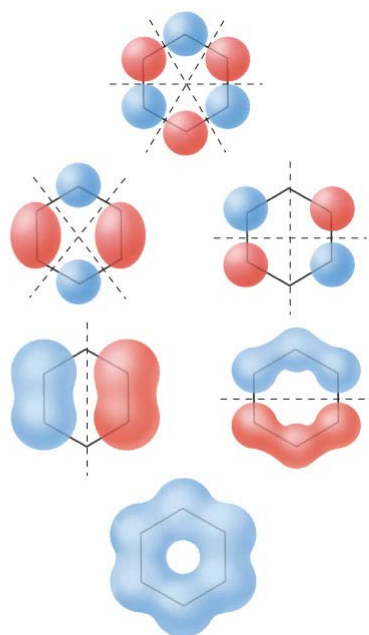
(d) The number of nodal planes increases with energy as in the particle-in-a-box problem. For each molecular orbital in the energy level diagram show the locations of nodes. If there is no node, write 'no node'. (3 pts) (0.5 pts each for correct node location, Maximum 3 pts)

Answer)

(c)



(d)

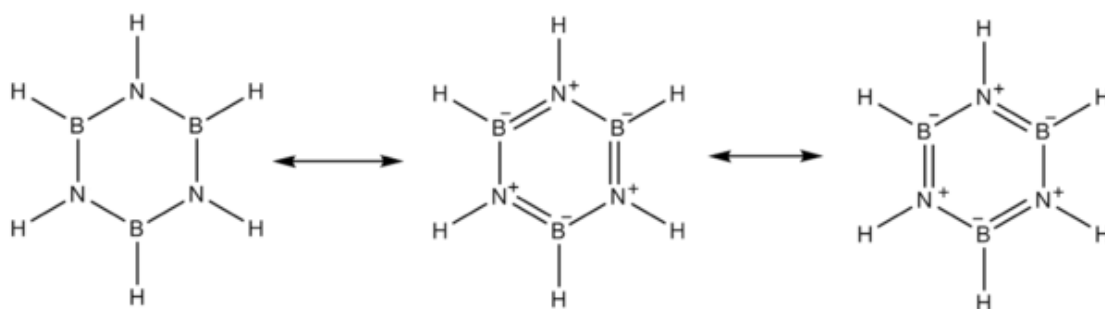


c) MO : 2 pts, electron configuration : 1 pt

d) Each 0.5 pts(The plane of benzene ring itself is a nodal plane, Dashed line above and interatomic plane of benzene ring must be shown.)

(e) Borazine, referred as “inorganic benzene”, is an inorganic compound with the chemical formula  $(\text{BH})_3(\text{NH})_3$ , three BH units and three NH units alternating. The boron-nitrogen bond length is between that of the boron-nitrogen single bond (0.151 nm) and the boron-nitrogen double bond (0.131 nm). Draw the all possible resonance hybrid Lewis diagrams of borazine and explain this result (boron-nitrogen bond length) with the Lewis diagram of borazine. (Show lone pairs and formal charge too.) (5 pts) (3 pts for all correct Lewis diagrams, -0.5 pts for incorrect formal charge, 2 pts for correct explanation)

Answer)



The low electronegativity of boron (2.04) compared to that of nitrogen and the electron deficiency on the boron atom makes nitrogen lone-pair electrons partially delocalized throughout six B-N bonds.

Lewis diagram : 3 pts (each 1 pt), formal charge error in each diagram : -0.5 pts, explanation 2 pts



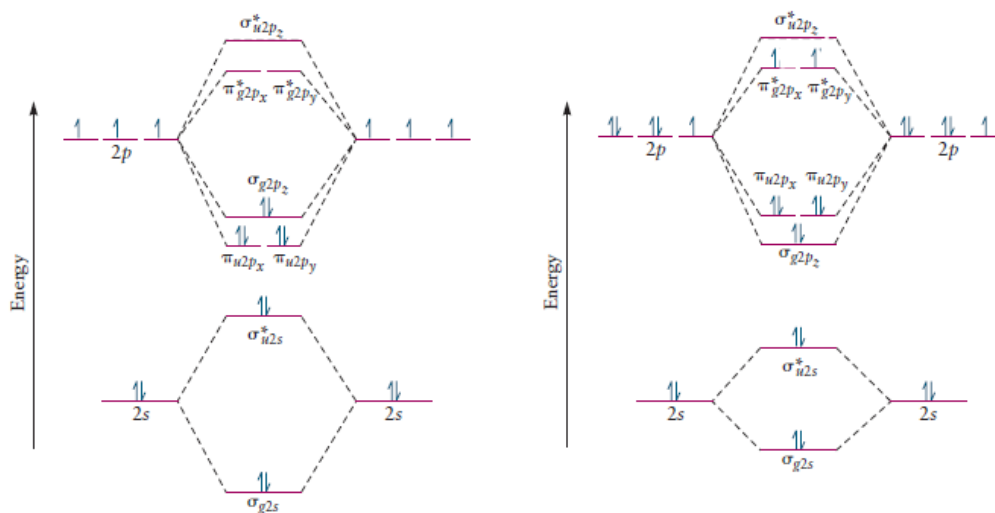
10. Answer the following questions (Total 10 pts)

(a) Determine the ground-state electron configuration and bond order of the  $N_2$  and  $O_2$  molecule from the correlation diagram for the molecules. (3 pts) (1 pt for each correlation diagram, 0.5 pts for each bond order)

Answer)

nitrogen molecule (left), oxygen molecule (right).

Bond order=3 for nitrogen molecule, 2 for oxygen molecule



Correlation diagram : 1 pt each, bond order : 0.5 pts each

(b) Explain about the difference in ordering energy of the molecules. (2 pts) (No partial pts)

Answer)

For homonuclear diatomic molecules of  $Z \leq 7$ , reversed ordering of energy occurs due to large electron-electron spatial repulsions between electrons in  $\sigma_{g2p_z}$  and  $\sigma_{u2s}^*$  MOs. For homonuclear diatomic molecules of  $Z > 7$ , it has normal ordering of energy because as  $Z$  increases, the repulsion decreases since electrons in  $\sigma_{g2s}$  and  $\sigma_{u2s}^*$  MO's are drawn more strongly toward the nucleus.

(c) Are molecular oxygen and molecular nitrogen paramagnetic or diamagnetic? (1 pt) (0.5 pts each)

Answer)

$N_2$  : Diamagnetic (No unpaired electrons)  $O_2$  : Paramagnetic (Unpaired electrons exist)

0.5 pts each

(d) Predict the order of the first ionization energy of molecular nitrogen, molecular oxygen, atomic nitrogen, and atomic oxygen. (4 pts) (1 pt for correct order, 3 pts for correct explanation)

Answer)

$O_2$  (1205 kJ/mol) < O (1313 kJ/mol) < N (1402 kJ/mol) <  $N_2$  (1503 kJ/mol)

In the correlation diagram of  $O_2$ , a 2p electron of a ground state of O atom lies lower in energy than the  $\pi_{g2p}^*$  electron, which is the highest energy electron in the ground state  $O_2$  molecule. Therefore, it requires more energy to ionize O than  $O_2$ . Similarly, for molecular nitrogen and atomic nitrogen, it requires less energy to ionize N than  $N_2$ . For nitrogen atom and oxygen atom, oxygen has small first ionization energy due to the repulsion between paired electrons in 2p orbitals.

Correct order : 1 pt, 1 pt for each correct explanation of order( $O_2 < O$ ,  $O < N$ ,  $N < N_2$ )