Write down your answers neatly in the spaces provided below the questions; print your
Student ID in the upper right-hand corner of every page.

** Professor Name  Class  Student I.D. Number  Name **

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** This paper consists of 14 sheets with 10 problems (pages 12 & 13 contain constants & the
periodic table; page 14 is the claim form). Please check all page numbers before taking the exam.
Write down your work and answers in the answer sheet.
Answers to numerical questions should include correct units: there is a 30% deduction for missing
or incorrect units.

** NOTICE: SCHEDULES on RETURN and CLAIM of the MARKED EXAM PAPER. **
1. Period, Location and Procedure
   1) Return and Claim Period: December 19 (Friday, 11:00-13:00, 2 hrs)
   2) Location: Creative Learning Bldg.(E11)
     
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3) Claim Procedure:
   Rule 1: Students cannot bring their own writing tools into the room.
   (Use a pen only provided by TA)
   Rule 2: With or without claim, you must submit the paper back to TA.
   (Do not go out of the room with it)
   (During the period, you can check the marked exam paper from your TA and should hand in the paper with a
FORM for claims if you have any claims on it. The claim is permitted only on the period. Keep that in mind! A
solution file with answers for the examination will be uploaded on 12/19 on the web.)

2. Final Confirmation
   1) Period: December 20(Sat) – 21(Sun)
   2) Procedure: During this period, you can check the final score of the examination on the website again.

   To get more information, visit the website at www.gencheminkaiast.pe.kr.
1. (a) Write structural formulas and name all the \textit{straight chain} alkenes with the molecular formula \( \text{C}_5\text{H}_{10} \). (5 points)

\begin{itemize}
  \item \( \text{H}_2\text{C} = \text{CH} - \text{CH}_2\text{CH}_2\text{CH}_3 \quad \text{1-pentene} \) (2 points)
  \item \( \text{H}_3\text{C} - \text{C} - \text{C} - \text{CH}_2\text{CH}_3 \quad \text{cis-2-pentene} \) (2 x 1.5 points)
  \item \( \text{H}_3\text{C} - \text{C} - \text{H} - \text{CH}_2\text{CH}_3 \quad \text{trans-2-pentene} \) (2 x 1.5 points)
\end{itemize}

(allow for different correct styles of structural formulas)

(b) Write the structural formula of all the \textit{structural (constitutional)} isomers that have the molecular formula \( \text{C}_5\text{H}_{10} \), but which are \textit{not} alkenes. (5 points)

\begin{itemize}
  \item \( \text{H}_2\text{C} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 \)
  \item \( \text{H}_2\text{C} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 \)
  \item \( \text{H}_2\text{C} - \text{CH}_3 - \text{CH}_3 - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 \)
  \item \( \text{H}_2\text{C} - \text{CH}_3 - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 - \text{CH}_2 - \text{CH}_3 \)
  \item \( \text{H}_2\text{C} - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 \)
\end{itemize}

(5 x 1 points)

(allow for different correct styles of structural formulas)

2. (a) Write the hybridization mode (sp\(^3\) etc) for each of the carbon atoms in 2,3-butadien-1-ol, below. (2 points)

\begin{itemize}
  \item \( \text{H} - \text{C} = \text{C} = \text{C} = \text{H} - \text{CH}_2\text{OH} \)
\end{itemize}

\textbf{(Answer)}

\begin{itemize}
  \item \( \text{sp}^2 \)
  \item \( \text{sp} \)
  \item \( \text{sp}^2 \)
\end{itemize}

\begin{itemize}
  \item \( \text{sp}^3 \) (2 points)
\end{itemize}

(b) Write balanced equations, showing structural formulas, for each of the following reactions.

(i) Dehydration of 3-heptanol to give 3-heptene. (1.5 points)

(ii) Dehydration of ethanol to give diethyl ether. (2.5 points)

(iii) Dehydrogenation of phenylmethanol (benzyl alcohol) to phenylmethanal (benzaldehyde). (1.5 points)

(iv) Bromination of propene and then dehydrobromination of the product to give 1-bromo-1-propene. (2.5 points)
3. (a) Write a chemical formula for each of the following compounds:
(i) ammonium diamminetetracyanochromate(III),
(ii) pentacarbonyltechnetium(I) iodide,
(iii) potassium pentacyanomanganate(IV),
(iv) tetra-ammineaquachloridocobalt(III) bromide

(Answer)
(a) (i) $\text{NH}_4[\text{Cr(NH}_3)_2\text{CN}]_4$
(ii) $[\text{Tc(CO)}_5]_1$
(iii) $K[\text{Mn(CN)}_5]$
(iv) $[\text{Co(NH}_3)_4\text{(H}_2\text{O)}\text{Cl}]\text{Br}_2$ (4 x 1 points)

(b) Sketch the structures of all the distinct isomers of the following two complexes indicating the types of isomers present in each case. (6 points)

(i) $[\text{Pt(NH}_3)_2\text{Br}_2]$
(ii) $[\text{Co(H}_2\text{O)}_3\text{(CN)}_2\text{Br}]^-$

(Answer)
(i) $\text{Br}_{\text{cis}}\text{Pt}\text{Br}_{\text{cis}}\text{NH}_3_{\text{cis}}\text{NH}_3_{\text{cis}}$

$\text{Br}_{\text{trans}}\text{Pt}\text{Br}_{\text{trans}}\text{NH}_3_{\text{trans}}$

$\text{cis isomer}$

$\text{trans isomer (geometric isomerism)}$

(ii) $\text{OH}_2\text{Br}\text{NC}_{\text{fac}}\text{Co}_{\text{fac}}\text{OH}_2$

$\text{Br}\text{OH}_2\text{NC}_{\text{trans}}\text{Co}_{\text{trans}}\text{OH}_2$

$\text{OH}_2\text{Br}\text{NC}_{\text{cis}}\text{Co}_{\text{cis}}\text{OH}_2$

$\text{fac isomer}$

$\text{trans mer isomer}$

$\text{cis mer isomer}$

Allow for alternative correct sketch styles
4. (a) Use crystal field theory to draw 'line and arrow' diagrams illustrating the $e_g$ and $t_{2g}$ electron configuration of the following, and state the number of unpaired electrons for each:

(i) Fe(H$_2$O)$_6^{2+}$ and Fe(CN)$_6^{4-}$
(ii) Fe(H$_2$O)$_6^{3+}$ and Fe(CN)$_6^{3-}$  (6 points)

(Answer)

(i) Fe(H$_2$O)$_6^{2+}$

4 unpaired electrons

(ii) Fe(H$_2$O)$_6^{3+}$

5 unpaired electrons

(b) Estimate the crystal field stabilization energy (in terms of $\Delta_o$) of the two configurations in (ii). (2 points)

(Answer)

(For Fe(H$_2$O)$_6^{3+}$ [(t$_{2g}$)$^3$ (e$_g$)$^2$]), CFSE = 0
(For Fe(CN)$_6^{3-}$ [(t$_{2g}$)$^5$]), CFSE = $2\Delta_o$  (2 x 1 points)

5. Chemical analysis of a newly discovered gaseous compound showed that it contained 33.0% silicon and 67.0% fluorine by mass. At 35.0 °C, 210 mL of the compound exerted a pressure of 1.72 bar. If 210 mL of the compound weighed 2.38 g, under these conditions, determine the molecular formula of this compound, assuming it behaves as an ideal gas. Show working. (10 points)

Molar masses (g mol$^{-1}$): Si = 28.09; F = 19.00.
R = 8.314 x 10$^{-2}$ L bar K$^{-1}$ mol$^{-1}$,
(Answer)
100.0 g of the compound contains 33.0 g Si and 67.0 g F, hence

No moles of Si = 33.0 g/28.09 g/mol = 1.17
No. moles of F = 67.0 g/19.00 g/mol = 3.53

Therefore the empirical formula is SiF₃. To find the molecular formula, use the ideal gas equation to compute molar mass via the number of moles corresponding to 2.38 g.

\[ pV = nRT \]
\[ n = \frac{(1.72 \text{ bar})(0.210 \text{ L})}{(8.314 \times 10^{-2} \text{ bar L/K mol})(308 \text{ K})} = 0.0141 \text{ mol} \]

Because there are 0.0141 mol in 2.38 g,

molar mass = \[ \frac{2.38 \text{ g}}{0.0141 \text{ mol}} = 169 \text{ g/mol} \]

Since the molar mass of the empirical formula is 85.1 g/mol, the molecular formula is twice the empirical formula, that is Si₂F₆

(10 points) (Allow partial points and alternative correct working)

6. Submarine design teams have investigated the use of potassium superoxide, KO₂, as an air purifier because this compound reacts with carbon dioxide and at the same time releases oxygen, according to the equation,

\[ 4\text{KO}_2(\text{s}) + 2\text{CO}_2(\text{g}) \rightarrow 2\text{K}_2\text{CO}_3(\text{s}) + 3\text{O}_2(\text{g}) \]

(a) Calculate the mass of KO₂ needed to react with 100 L of CO₂ at 25.0 °C and 1.03 atm, and the volume of O₂ released under these conditions. Show working. Both gases can be considered to be ideal. (8 points)

[R = 0.0821 L atm K⁻¹ mol⁻¹. Molar masses (g mol⁻¹): K = 39.1; O = 16.0]

(Answer)
(a) Since CO₂ can be considered to behave ideally,

\[ PV = nRT \]
\[ (1.03 \text{ atm})(100 \text{ L}) = n(0.0821 \text{ L atm /Mol K})(298 \text{ K}) \]

No. moles of CO₂ absorbed = 4.21
Hence no. moles of KO₂ reacted = 8.42

\[ \therefore \text{Mass of KO}_2 \text{ reacted} = (8.42 \text{ mol})(71.1 \text{ g/mol}) \]
\[ = 599 \text{ g} \] (5 points)

No. moles and volume of O₂ = 3/2 x no. moles and volume of CO₂ (under same consitions)
Hence Volume of O₂ released = 150 L (3 points)

Allow for alternative correct working and allow partial points
(b) State whether more or less KO$_2$ would be needed to absorb the same volume of CO$_2$ at 1.03 atm and 30.0 °C. (2 points)

(Answer)

Less (2 points)

7. (a) Identify the major attractive force(s) that exist in associations amongst particles of the following substances:

(i) Cl$_2$ (liquid)  (ii) SO$_2$ (liquid)  (iii) KH (solid)  (iv) CuSO$_4$.5H$_2$O (solid)  (6 points)

(Answer)

(a) (i) London dispersion force (1 point)
(ii) Dipole-dipole force and London dispersion force (1 point)
(iii) Ionic (electrostatic or Coulombic) force (1 point)
(iv) Ionic (electrostatic or Coulombic) force, ion-dipole force (or covalent force) and hydrogen bonding (3 points)

(b) Acetic acid (CH$_3$COOH) exists as hydrogen bonded dimers in nonpolar solvents such as carbon tetrachloride. Draw a suitable structure for the dimer and state which intermolecular force is mainly responsible for holding the two monomers together in the dimer. (3 points)

(Answer)

(b)

\[
\begin{array}{c}
\text{O} \quad \text{H} \quad \text{O} \\
\text{C} \quad \text{H} \quad \text{C} \\
\text{O} \quad \text{H} \quad \text{O}
\end{array}
\]  (2 points)

The major intermolecular force is hydrogen bonding (1 point)

(Allow partial points)

State whether these dimers are likely to exist in aqueous solutions of acetic acid (yes or no). (1 point)

(Answer)

No (1 point)
8. Study the phase diagram for carbon dioxide below and answer the following questions.

(i) Identify points C, B, and A. (3 points)
(ii) Summarize the general properties of carbon dioxide at temperatures above 303.2 K and pressures above 73.5 bar. (2 points)
(iii) Describe the sequence of events that occur when carbon dioxide at 2 bar pressure is heated to 273 K. (2 points)
(iv) Describe the sequence of events that occur when carbon dioxide at 70 bar pressure is heated to 273 K. (2 points)

(Answer)

(i) C is the (normal) sublimation point; B is the triple point; A is the supercritical point (3×1 points)
(ii) Under these conditions carbon dioxide is a supercritical fluid; its properties are intermediate between those of a gas and a liquid (it flows, but has no meniscus). (2 points)
(iii) Solid is converted directly to vapor (it sublimes), at the temperature given at the interception of the 2 bar constant pressure line with the solid-vapor curve. (2 points)
(iv) Solid melts at the intercept of the 70 bar constant pressure line with the solid-liquid curve and the liquid vaporizes at the intercept with the liquid-vapor curve. (2 points)

9. A solution of hydrobromic acid in water is 48.30% HBr by mass. Its density is 1.488 g/cm³ at 20 °C. Compute the concentration of HBr in terms of molarity, molality, and mole fraction, at this temperature. (10 points)

[| Molar masses (g/mol) | H | Br | O |
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(Answer)
Exactly 100 g of solution contain 48.30 g HBr and 51.70 g water

Its volume is \[ 100 \text{ g} \times \left( \frac{1 \text{ mL soln}}{1.488 \text{ g soln}} \right) = 67.20 \text{ mL} \]

No. Moles HBr = \[ 48.30 \text{ g HBr} \left( \frac{1 \text{ mol}}{80.91 \text{ g}} \right) = 0.5970 \]

No. moles water = \[ 51.70 \text{ g water} \left( \frac{1 \text{ mol}}{18.02 \text{ g}} \right) = 2.869 \]

Molarity of HBr = \[ \frac{0.5970 \text{ mol}}{67.20 \text{ mL}} \left( \frac{1000 \text{ mL}}{1 \text{ L}} \right) = 8.884 \text{ mol/L (or M)} \]

Molality of HBr = \[ \frac{0.5970 \text{ mol}}{51.70 \text{ g}} \left( \frac{1000 \text{ g}}{1 \text{ kg}} \right) = 11.55 \text{ mol/kg (or m)} \]

Mole fraction of HBr = \[ \frac{0.5970 \text{ mol}}{0.5970 + 2.869 \text{ mol}} = 0.1722 \]

Allow partial points and correct alternative working

10. (a) When an unknown non-volatile hydrocarbon (5.50 g) is dissolved in benzene (100.0 g), the boiling point increases by 0.903 °C. If the boiling point elevation constant (ebullioscopic constant, \( K_b \)) for benzene is 2.53 K kg mol\(^{-1} \), determine the molar mass of the unknown hydrocarbon. Show working. (6 points)

(Answer)

(a) \[ \Delta T_b = K_b m \]

\[ m = \frac{0.903 \text{ K}}{2.53 \text{ K kg/mol}} = 0.357 \text{ mol/kg} \]

This corresponds to \[ 0.357 \text{ mol/kg} \times \frac{100 \text{ g}}{1000 \text{ g/kg}} \text{ mol} \]

= \[ 3.57 \times 10^{-2} \text{ mol} \]

Since no. moles = \[ \frac{\text{mass (g)}}{\text{molar mass M (g/mol)}} \]

\[ M = \frac{5.50 \text{ g}}{3.57 \times 10^{-2} \text{ mol}} \]

= \[ 154 \text{ g/mol} \]

(6 points)(Allow partial points)
(b) Study the temperature versus mole fraction diagram below for the binary acetone/chloroform solution and answer the following questions.

(i) Identify the points A, B, and C. (3 points)
(ii) Explain what happens when a solution of composition X (0.25 mole fraction of chloroform and 0.75 mole fraction of acetone) is distilled. (3 points)

(Answer)

(b) (i) A is the boiling point of pure chloroform; B is the boiling point of pure acetone; C is the boiling point of the azeotropic (constant boiling) mixture. (3 x 1 points)

(ii) Pure acetone distills first so the liquid in the flask will become gradually depleted in acetone and richer in chloroform until the composition of the liquid reaches 0.66 mole fraction of chloroform and 0.34 mole fraction of acetone. At this point the temperature rises to 64.7 °C and the azeotropic mixture distills until the flask is empty. (3 points)
Write down your answers neatly in the spaces provided below the questions; print your Student ID in the upper right-hand corner of every page.

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** This paper consists of 12 sheets with 11 problems (pages 10 & 11 contain constants & the periodic table; page 12 is the claim form). Please check all page numbers before taking the exam. Write down your work and answers in the answer sheet. Answers to numerical questions should include correct units: there is a 30% deduction for missing or incorrect units.

NOTICE: SCHEDULES on RETURN and CLAIM of the MARKED EXAM PAPER.

1. Period, Location, and Procedure
Return and Claim Period: **Monday October 27 (18:30 ~ 19:30)**
Location: **Room for quiz session**
Procedure: **Rule 1:** Students cannot bring their own writing tools into the room. (Use a pen only provided by TA) **Rule 2:** With or without claim, you must submit the paper back to TA. (Do not leave the room with it).
If you have any claims, you can submit the claim paper with your opinion. After writing your opinions on the claim form, attach it to your mid-term paper with a stapler. Give them to TA.
(Note: the claim is permitted only during this period. A solution file with answers for the examination will be uploaded on 10/26 on the web.)

2. Final Confirmation
Period: **Thursday 30 October- Friday 31 October**
Procedure: During this period, you can check final score of the examination on the website again.

** For further information, please visit General Chemistry website at [www.gencheminkaist.pe.kr](http://www.gencheminkaist.pe.kr).
1. (a) Determine which one in each of the following pairs has the higher first ionization energy. (4 points)

(i) Cs or Ba  (ii) Tl or Bi  (iii) Xe or Cs  (iv) Ge or Pb

Answer

(i) Ba  (ii) Bi  (iii) Xe  (iv) Ge  (4 x 1 points)

(b) Arrange the following in order of bond strength. (4 points)

(i) H₂Se; H₂S; H₂Te
(ii) O₂; F₂; N₂
(iii) The CO bond in H₂CO; CO; CO₂

Answer

(i) H₂S > H₂Se > H₂Te (1 point)
(ii) F₂< O₂< N₂ (1 point)
(iii) CO > CO₂ > H₂CO (2 points)

(c) Explain briefly why the bond length of H₂ (0.75 Å) is approximately twice the atomic radius of H (0.37 Å), whereas the bond length of F₂ (1.42 Å) is considerably longer than twice the atomic radius of F (0.64 Å). (2 points)

Answer

Lone pair-lone pair repulsion on opposite F atoms in F₂ results in a longer than expected F-F bond distance, so as to minimize repulsion. No such repulsions exist in H₂. (3 points) (Allow other correct explanation)

2. The diagram below illustrates the potential energy versus distance relationships for Na and Cl atoms and also for Na⁺ and Cl⁻ ions (all in the gas phase).
(a) Identify the curve A. (1 point)
(b) Identify the curve B. (1 point)
(c) What is the distance C? (1 point)
(d) Identify the energy D. (1 point)
(e) What is the energy E? (2 points)

Answer

(a) Na⁺ + Cl⁻ (1 point) [can include (g)]
(b) Na + Cl (1 point) [can include (g)]
(c) The optimum distance for Na⁺Cl⁻ (1 point)
(d) The bond dissociation energy of Na⁺Cl⁻ (1 point)
(e) Ionization energy of Na minus the electron affinity of Cl (2 points)

3. (a) Write a Lewis structure for carbon monoxide, showing formal charges. (2 points)

Answer

\[ \text{C} = \text{O} \] (2 points)

(b) Write a Lewis structure for carbon monoxide that shows partial charge separation (δ⁺, δ⁻), according to electronegativities. (2 points)

Answer

\[ \delta^+ \quad \delta^- \] \[ \text{C} = \text{O} \] (2 points)

(c) Use your answer in (a) and (b) to predict the size of the dipole moment of carbon monoxide as zero, small, or large. (2 points)

Give a brief explanation. (2 points)

Answer

Small (2 points). The formal charge allocation and electronegativity partial separation oppose each other. (2 points)

4. For nitrogen tetraoxide, write the best Lewis (resonance) structures, with formal charges, assuming there is an N-N bond. (6 points)

Answer

\[ \text{Answer} \]

\[ (\text{4 x 1.5 points}) \]
5. (a) Use the Bohr model to determine the excited electronic state of B$^{4+}$ that has the same energy as the ground state of hydrogen. (6 points)

[R$_H$ (Rydberg constant) = 3.29 x 10$^{15}$ m$^{-1}$; c (speed of light) = 3.00 x 10$^8$ m/s; h (Planck’s constant) = 6.626 x 10$^{-34}$ Js]

**Answer**

For H, Z = 1 and for B$^{4+}$, Z = 5.
The energy of electronic levels is given in rydbergs by

\[ E_n = -\frac{Z^2}{n^2} \]

For the ground state of H, n = 1, hence

\[ \left( -\frac{Z^2}{n_1^2} \right)_H = \left( -\frac{Z^2}{n_1^2} \right)_{B^{4+}} \]

or

\[ -\frac{1}{1} = -\frac{25}{n_5^2} \]

\[ n_5^2 = 25 \]

n = 5 (\(= 4^{th}\) excited state) (5 points)

(b) B$^{4+}$ ions have been observed in the atmospheres of stars.
Use the Bohr model to calculate the wavelength (in nm) of the light emitted in a transition from the n = 5 state to the n = 1 state of this ion. (4 points)

[speed of light in vacuum = 2.998 x 10$^8$ m s$^{-1}$, Planck’s constant = 6.626 x 10$^{-34}$ Js, 1 rydberg = 2.180 x 10$^{-18}$ J]

**Answer**

\[ \Delta E = E_{n5} - E_{n1} = \left( -\frac{25}{25} + \frac{25}{1} \right) \text{(rydbergs)} (2.180 \times 10^{-18} J/ \text{rydberg}) \]

\[ = 5.232 \times 10^{-17} J \]

Since \( \Delta E = \frac{hc}{\lambda} \),

\[ 5.232 \times 10^{-17} J = \frac{(6.626 \times 10^{-34} J s)(2.997 \times 10^8 \text{ m s}^{-1})}{\lambda (\text{m})} \]

\[ \lambda = 3.796 \times 10^{-9} \text{ m} = 3.796 \text{ nm} \] (4 points)

6. (a) The diagram below shows the allowed energies of a particle in a one-dimensional box of 1 unit length (L = 1), in units of $\hbar^2/8m$. In the space to the right sketch the positions of the corresponding energy levels for a particle in a one-dimensional box of 2 units length (L = 2). (3 points)
(b) Write the equation for the energy of a particle in a two-dimensional box of sides L (a square box). (2 points)

Answer

\[ E = \frac{\hbar^2}{8mL^2} \left( n_1^2 + n_2^2 \right) \], where \( n_1 = 1, 2, 3, \ldots \) and \( n_2 = 1, 2, 3, \ldots \)  

(2 points)

(or \( E_{n_1,n_2} \))

(c) Assuming that the energy levels are not influenced by repulsion between multiple electrons, use the Aufbau Principle (and associated principles and rules) to draw a ‘line and arrow’ diagram of the ground state electronic configuration for four electrons in the box. (3 points)

Answer

\[ E_{1,1} \]

\[ E_{1,2} = E_{2,1} \]

(3 points)

7. Study the following hydrogen atom wave functions (b)- (e) and fill in the spaces in the box below. The answer for (a) is given as an example (10 points)
(a) $\psi_{nlm} = \frac{1}{4\sqrt{2\pi}} \frac{-3/2}{a_0} \int \frac{-i/2a_0}{a_0} \sin \theta \cos \phi$

(b) $\psi_{nlm} = \frac{1}{8\sqrt{6\pi}} a_0^{-3/2} \left( \frac{r}{a_0} \right)^2 e^{-r/3a_0} (3\cos^2 \theta - 1)$

(c) $\psi_{nlm} = \frac{1}{81\sqrt{6\pi}} a_0^{-3/2} (27 - 18r/a_0 + 2r^2/a_0)^2 e^{-r/3a_0}$

(d) $\psi_{nlm} = \frac{1}{4\sqrt{2\pi}} a_0^{-3/2} \frac{-r/2a_0}{a_0} \cos \theta$

(e) $\psi_{nlm} = \frac{1}{512\sqrt{5\pi}} a_0^{-3/2} \left( 80 - \frac{20r}{a_0} + \frac{r^2}{a_0} \right) e^{-r/4a_0} \sin \theta \sin \phi$

**Answer**

<table>
<thead>
<tr>
<th>Orbital</th>
<th>Name</th>
<th>n, l, m values</th>
<th>No. radial nodes</th>
<th>No. angular nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>2p_x</td>
<td>2, 1, +1 (or – 1)</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>(b)</td>
<td>3d_z2</td>
<td>3, 2, 0</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>(c)</td>
<td>3s</td>
<td>3, 0, 0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>(d)</td>
<td>2p_z</td>
<td>2, 1, 0</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>(e)</td>
<td>4p_y</td>
<td>4, 1, +1 (or – 1)</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

(4 x 2.5 = 10 points)

8. The Photoelectron spectrum of atomic fluorine shows ionization energies of 689 eV, 34 eV and 12 eV. Assign these energies to the orbitals of F (3 points) and estimate the value of $Z_{\text{eff}}$ for F for each of these orbitals. (6 points) Assume 1 rydberg = 13.61 eV.

**Answer**

According to Koopman's approximation, the orbital energies are: -689 eV, -34 eV, and -12 eV; corresponding to 1s, 2s and 2p orbitals, respectively. (3 points)

$E_n \sim -\frac{Z_{\text{eff}}^2}{n^2}$ or $Z_{\text{eff}} \sim \sqrt{-E_n n^2}$, where $E_n$ is in rydbergs

$Z_{\text{eff}}(1s) = \sqrt{(+689 \text{ eV})(1^2)} = 7.12$  $Z_{\text{eff}}(2s) = \sqrt{(+34 \text{ eV})(2^2)} = 3.16$

$Z_{\text{eff}}(2p) = \sqrt{(+12 \text{ eV})(2^2)} = 1.88$ (3 x 2 points)
9. The dioxygen species $O_2^+$, $O_2$, $O_2^-$ and $O_2^{2-}$ are all known and are well characterized.
(a) Construct a full LCAO-MO correlation diagram for $O_2^-$. (6 points)

Answer

(b) Write the electronic configuration of $O_2^+$. (2 points)

Answer

(c) Determine the bond order for $O_2^+$, $O_2$, $O_2^-$ and $O_2^{2-}$. (2 points)

Answer

10. (a) Draw the best Lewis structures for the nitrite ion (NO$_2^-$). (2 points)

Answer

(b) Use the VSEPR theory to determine the steric number of N and the shape of the ion. (2 points)

Answer

Steric number of N = 3; V-shape (or bent) (2 points)
(c) For just one of the structures in (a), sketch the valence bond (VB) description of bonding, showing clearly the hybridization on N, the $\sigma$ and $\pi$ bonds, and lone pair electrons. (5 points)

**Answer**

![Valence bond diagram](image)

(d) Sketch the $\pi$ molecular orbitals and $\pi$ MO correlation diagram for NO$_2^-$: (5 points)

**Answer**

![MO diagram](image)

11. Determine whether the following statements are true or false. Write T or F in the boxes adjacent to the questions. (10 points)

(a) According to the Aufbau Principle, 5g orbitals will be occupied in the 8th period.  

(b) Fluorine is the most electronegative element, but its electron affinity is somewhat smaller than chlorine’s due to the small size of fluorine’s orbitals.

(c) The 3rd row D-block elements have similar atomic radii to those of the 2nd row D-block elements.

(d) Both Sc and Sc$^+$ are paramagnetic.
(e) The sulfur trioxide (SO₃) molecule is tetrahedral and highly polar.  

(f) For the B atom, the principal quantum number (n) completely defines the energy of a given electron, whereas n and ℓ (the angular momentum quantum number) are both needed to define the energy of a given electron in B⁴⁺.

(g) The allowed energy levels of an electron in a box are lower and more closely spaced than those of an electron in a small box.

(g) The normalization constant of a wave function is calculated by setting to 1 the integral of the wave function over all space.

(h) According to LCAO-MO theory, the Be₂⁺ molecular ion has stronger bonding than the Be₂ molecule.

(i) According to VB theory, the molecule CH₃-CH=C=CH₂ has sp, sp² and sp³ hybridized C atoms.