(一) **Multiple choice (there is only one correct answer for each question) (60 pts.).** 單選題；答錯不倒扣

1. Treatment of cyclopentene with peroxybenzoic acid _____.

(a) results in oxidative cleavage of the ring to produce an acyclic compound.

(b) yields a meso epoxide. (c) yields an equimolar mixture of enantiomeric epoxides.

(d) gives the same product as treatment of cyclopentene with OsO_4.

(e) none of the above.

2. Addition of Br_2 to (*E*)-hex-3-ene produces _____.

(a) a meso dibromide. (b) a mixture of enantiomeric dibromides which is optically active.

(c) a mixture of enantiomeric dibromides which is optically inactive.

(d) (*Z*)-3,4-dibromo-3-hexene. (e) (*E*)-3,4-dibromo-3-hexene.

3. Which of the following additions to alkenes occur(s) specifically in an anti fashion?

(a) hydroboration-oxidation. (b) addition of Br_2. (c) addition of H_2.

(d) addition of H_2O in dilute acid. (e) both A and B.

4. Which of the following additions to alkenes occur(s) specifically in an syn fashion?

(a) dihydroxylation using OsO_4, H_2O_2. (b) addition of $H_{2/Pt}$. (c) hydroboration.

(d) addition of HCl. (e) a, b, and c.

5. HBr can be added to an alkene in the presence of peroxides (ROOR). What function does the peroxide serve in this reaction?

(a) nucleophile. (b) electrophile. (c) radical chain initiator. (d) acid catalyst. (e) solvent.

6. When an alkene is subjected to treatment with $Hg(OAc)_2$ in alcohol followed by reaction with $NaBH_4$, what new class of compound is formed?

(a) ether. (b) epoxide. (c) alkane. (d) syn diol. (e) alkyne.

7. Treatment of 2-methylpropene with which of the following reaction conditions results in an anti-Markovnikov addition product?

(a) dry gaseous HBr with peroxides present. (b) BH_3-THF, followed by alkaline H_2O_2.

(c) aqueous $Hg(OAc)_2$, followed by alkaline $NaBH_4$. (d) dilute H_2SO_4 and heat.

(e) both A and B.

8. Which of the following reagents should be used to convert hex-3-yne to (*Z*)-hex-3-ene?

(a) H_2, Pt. (b) Na, NH_3. (c) H_2, Lindlar's catalyst. (d) H_2SO_4, H_2O. (e) $HgSO_4$, H_2O.

9. What is the major organic product that results when 1-heptyne is treated with 2 equivalents of HBr?

(a) 2,3-dibromo-1-heptene. (b) 2,3-dibromo-2-heptene. (c) 1,2-dibromoheptane.
(d) 2,2-dibromoheptane. (e) 1,1-dibromoheptane.

10. Which of the following alkyl halides would be suitable to use when forming a Grignard reagent?
(a) $BrCH_2CH_2CH_2CN$. (b) $CH_3COCH_2CH_2Br$. (c) $(CH_3)_2NCH_2CH_2Br$. (d) $H_2NCH_2CH_2Br$.
(e) all of the above.

11. Which of the following terms best describes the reactive nature of a Grignard reagent?
(a) carbocation. (b) free radical. (c) electrophile. (d) nucleophile. (e) carbene.

12. Which of the following alcohols will give a positive chromic acid test?
(a) *tert*-butanol. (b) cyclohexanol. (c) pentan-3-ol. (d) both A and B. (e) both B and C.

13. Which of the following alcohols will react most rapidly with the Lucas reagent (HCl, $ZnCl_2$)?
(a) $(CH_3)_3COH$. (b) $CH_3CH_2CH_2CH_2OH$. (c) $CH_3CH(OH)CH_2CH_3$.
(d) $(CH_3)_2CHCH_2OH$. (e) $CH_2CHCH_2CH_2OH$.

14. Which of the following is not a true statement?
(a) Dioxanes are six-membered ring ethers. (b) Furans are five-membered ring ethers.
(c) Oxiranes are three-membered ring ethers. (d) Oxetanes are five-membered ring ethers.
(e) Pyrans are six-membered-ring ethers.

15. What compound is formed when ethylene oxide is reacted with n-pentyllithium followed by treatment with aqueous acid?
(a) 1-heptanol. (b) 2-heptanol (c) heptanal. (d) 2-heptanone. (e) pentanal

16. What is the hybridization of the central carbon of allene (1,2-propadiene)?
(a) sp. (b) sp^2. (c) sp^3. (d) p. (e) none of the above.

17. Which of the following molecules is chiral?
(a) 1,2-pentadiene . (b) 2,3-pentadiene . (c) 2-methyl-2,3-pentadiene
(d) 2-chloro-4-methyl-2,3-pentadiene . (e) none of the above molecules is chiral

18. Which of the following compounds is the most reactive dienophile in a Diels-Alder reaction with 1,3-butadiene?
(a) $CH_2=CHOCH_3$. (b) $CH_2=CHCHO$. (c) $CH_3CH=CHCH_3$. (d) $(CH_3)_2C=CH_2$
(e) $CH_2=CH_2$

19. Absorption of UV-visible energy by a molecule results in:
(a) vibrational transitions . (b) electronic transitions . (c) rotational transitions
(d) nuclear transitions . (e) none of the above

20. Which of the following compounds has the most negative heat of hydrogenation?
(a) 1,4-hexadiene . (b) 1,5-hexadiene . (c) 1,2-hexadiene . (d) 1,3-hexadiene . (e) hex-1-ene

21. Which of the following compounds has the most signals in the noise-decoupled ^{13}C NMR spectrum?
(a) *o*-dibromobenzene. (b) *m*-dibromobenzene. (c) *p*-dibromobenzene. (d) 1,3,5-tribromobenzene.
(e) 1,2,3,4-tetrabromobenzene.

22. Which of the following is the same as the tropylium ion?
(a) cycloheptatrienyl cation. (b) cycloheptatrienyl anion. (c) cyclopentadienyl cation.
(d) cyclopentadienyl anion. (e) cyclopropenyl anion

23. In electrophilic aromatic substitution reactions a bromine substituent:
(a) is a deactivator and a m-director. (b) is a deactivator and an o,p-director.
(c) is an activator and a m-director. (d) is an activator and an o,p-director.
(e) none of the above.

24. What intermediate is thought to occur in the elimination-addition nucleophilic aromatic substitution mechanism?
(a) radical anion. (b) radical cation. (c) quinine. (d) benzyne. (e) positively charged sigma complex.

25. The proton NMR spectrum of an unknown compound contains a triplet at 9.8 ppm. Which of the following could be this unknown?
(a) $(CH_3)_3CCHO$. (b) $CH_3CH_2CH_2CO_2H$. (c) $CH_3CH_2CH_2CHO$. (d) $CH_3CO\ CH_2Ph$. (e) PhCHO

26. The Hofmann elimination proceeds via a(n) _____ pathway.
(a) E2. (b) E1. (c) S_N1. (d) S_N2. (e) none of the above

27. Which of the following is not an alkaloid?
(a) cocaine. (b) mesitylene. (c) nicotine. (d) mescaline. (e) morphine

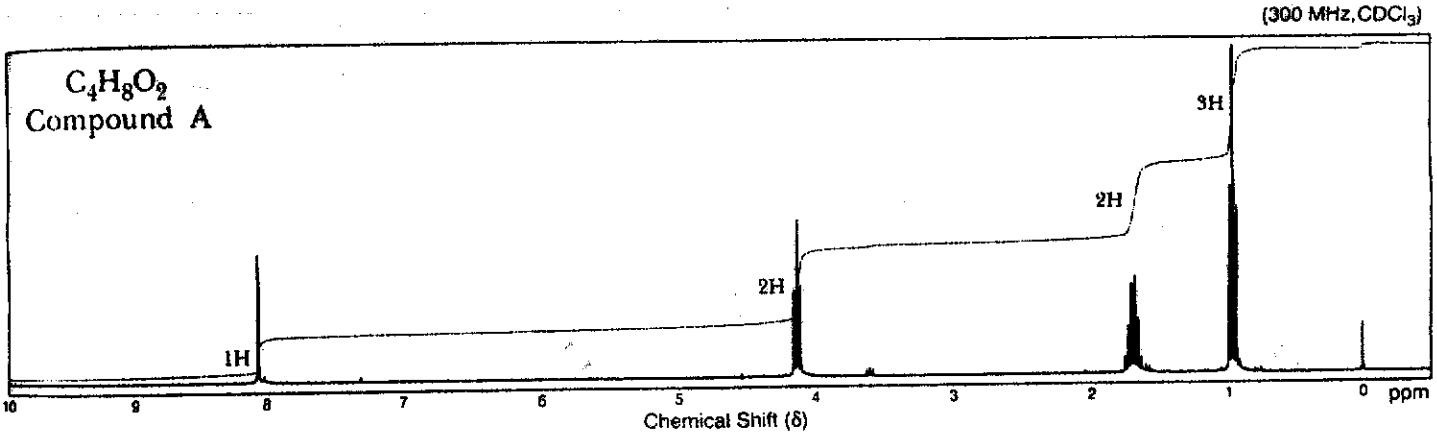
28. Which of the following conditions will drive the equilibrium of the Fischer esterification towards ester formation?
(a) addition of water. (b) removal of water as it is formed. (c) addition of an inorganic acid as a catalyst.

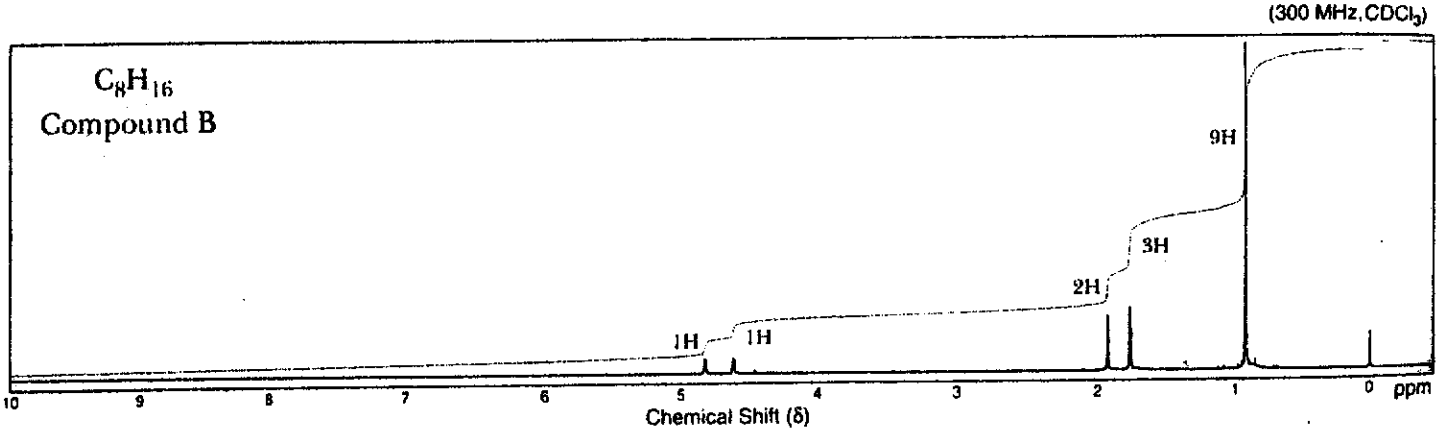
(d) addition of alcohol. (e) both B and D

29. Esters and amides are most easily made by nucleophilic acyl substitution reactions on:
(a) alcohols. (b) acid anhydrides. (c) carboxylates. (d) carboxylic acids. (e) acid chlorides

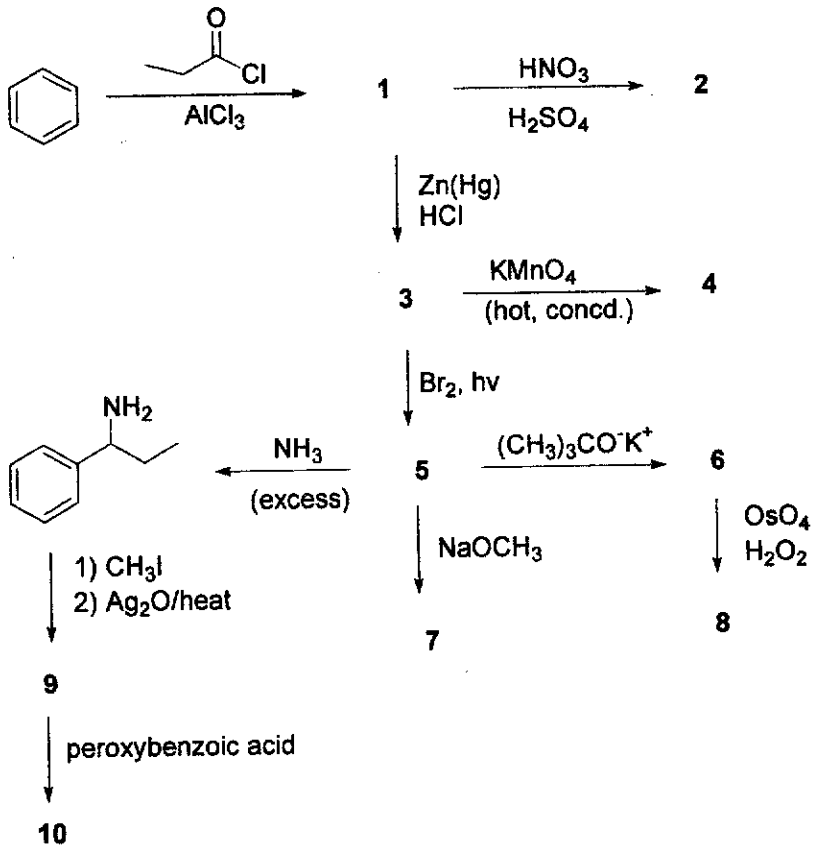
30. Acids can be reduced to aldehydes by:
(a) treatment with $LiAlH_4$.
(b) conversion to the acid chloride followed by treatment with $LiAlH[OC(CH_3)_3]_3$.
(c) conversion to the amide followed by treatment with $NaBH_4$.
(d) conversion to the ester followed by treatment with $LiAlH_4$.
(e) conversion to the anhydride followed by treatment with Mg and H_3O+.

(二) Based on the NMR spectra and molecular formula shown below. Propose structural formulas for compounds A and B (10 pts.).

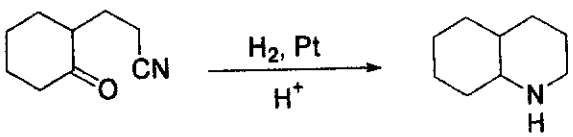




(三) Give the structures of the compounds 1 through 10 in the following series of reactions (20 pts.).



(四) Give reasonable mechanism for each of the following reactions (10 pts.).

1) 

2) $RCO_2H + CH_2N_2 \longrightarrow RCO_2CH_3$

I. 單選題 (共60分；每題4分，不倒扣)

1. Which of the following aqua acids has the lowest *pKa* value?
   (A) $[Fe(OH_2)_6]^{3+}$ (B) $[Fe(OH_2)_6]^{2+}$ (C) $[Sc(OH_2)_6]^{3+}$ (D) $[Cd(OH_2)_6]^{2+}$ (E) $[Al(OH_2)_6]^{3+}$

2. Which of the following is the correct description about $[Mo_2(\mu\text{-}SO_4)_4]^{3-}$ dimeric anion?
   (A) It's diamagnetic with one δ bond.
   (B) The bond order is 3 and spin multiplicity is 0.
   (C) The bond order is 3.5 and the Mo-Mo distance is shorter than that of $[Mo_2(\mu\text{-}SO_4)_4]^{2-}$.
   (D) The molecular shape is tetragonal prismatic and the oxidation state of Mo is +1.5
   (E) The electronic configuration is $\sigma^2\pi^4\delta^2$ and it is paramagnetic

3. Which of the following complex do not obey 18-electron rule?
   (A) $[Fe(NO)(CN)_5]^{4-}$ (with bent M-NO) (B) $[V(C_6H_6)(CO)_3]^{1-}$
   (C) $[Co(NH_3)_4(H_2O)(Cl)]^{2+}$ (D) $[Fe(C_5H_5)(CO)_2Br]^{+}$
   (E) $Mn(CH_3)(en)(CO)_3$ (where en = ethylenediamine)

4. Which of the following complex is isolobal with cyclopropane?
   (A) $[Os(CO)_4(\eta^2\text{-}C_2H_4)]_3$ (B) $[Co(CO)_3]_3$ (C) $[Ni(CO)_3]_3$
   (D) $[Co(CO)_4]_3$ (E) $[Fe(CO)_4]_3$

5. Select the <u>correct</u> statement for the kinetics of the following complexes:
   (A) $[Fe(NO_2)_6]^{4-}$ is more labile than $[FeF_6]^{4-}$ (B) $[V(H_2O)_6]^{2+}$ and $[Cr(H_2O)_6]^{2+}$ are both inert
   (C) $[Fe(CN)_6]^{4-}$ and $[FeF_6]^{4-}$ are both labile (D) $[Co(NH_3)_6]^{2+}$ is more labile than $[Co(NH_3)_6]^{3+}$
   (E) None of the above

6. Boranes with formula $B_nH_n^{4-}$ have
   (A) *n* bonding orbitals and *n* antibonding orbitals
   (B) total of *4n+4* bonding electrons
   (C) *n*+1 framework bonding orbitals
   (D) *arachno* boranes as its isomers
   (E) framework with *n* corners of (*n*+2)-cornered polyhedron

7. Which of the following ion <u>does not</u> show inert pair effect?
   (A) Sn^{+2} (B) Ga^{+3} (C) Tl^{+1} (D) Bi^{+3} (E) Pb^{+2}

8. Which of the following statement is <u>not correct</u>?
   (A) Pure silicon is an intrinsic semiconductor at room temperature.
   (B) Metal has fully filled conduction band.
   (C) The conductance of metal decreases with increasing temperature.
   (D) Adding phosphorus (P) in silicon makes an *n*-type of semiconductor
   (E) The *p*-type dopant has fewer valence electrons than the host.

9. The enthalpy change for a reaction can be obtained by:
   (A) slope from plot of $ln(1/K_{eq})$ vs. T (B) slope from plot of lnK_{eq} vs. T
   (C) slope from plot of $ln(1/K_{eq})$ vs. $1/T$ (D) slope from plot of lnK_{eq} vs. $1/T$
   (E) $-RTlnK_{eq}$

10. In a $[CoF_6]^{3-}$ complex the pairing energy of the electrons is 21000 cm^{-1} and the ligand field splitting is 13000 cm^{-1}. What should the spin-only magnetic moment (μ_s) be for this complex?
(A) 5 BM (B) 0 BM (C) 6 BM (D) 4BM (E) 2 BM

11. The ground state term symbol for high spin d^4 configuration in O_h symmetry is:
(A) ^5D (B) ^1S (C) ^3H (D) ^3P (E) ^6S

12. The point group for molecular C_{60} is: (A) O_h (B) C_1 (C) $D_{\infty h}$ (D) C_{5v} (E) I_h

13. Which is the correct statement concerning crystal structure of NaCl:
(A) Coordination number for either Na^+ or Cl^- is 6. (B) $r_+/r_- \leqq 0.414$
(C) The unit cell is body centered. (D) The unit cell is face centered. (E) None of the above

14. Which of the following complexes has the lowest LMCT band?
(A) $[Co(NH_3)_5F]^{2+}$ (B) $[Co(NH_3)_5Br]^{2+}$ (C) $[Co(NH_3)_5Cl]^{2+}$ (D) $[Co(NH_3)_5I]^{2+}$
(E) All shows the same LMCT band due to leveling effect from the solvent

15. Which of the following statements about molecular orbital is <u>not</u> correct?
(A) The HOMO for N_2 molecule is the $\sigma_g(2p)$. (B) The LUMO for O_2 molecule is the $\sigma_u^*(2p)$.
(C) The HOMO electrons of O_2 are paired. (D) The HOMO electrons of N_2 are paired.
(E) The LUMO of N_2 is higher in energy than the HOMO of O_2.

II. 是非題 (共 20 分)
(判斷下列敘述是否正確，對則寫"T"，錯則寫"F"；答對每題 2 分，<u>答錯每題倒扣 2 分</u>)

1. Hardness of a chemical species is defined as $(I-A)/2$ where I is the ionization energy and A is the electron affinity of that species.
2. The bond angles in PH_3 are larger than that in NH_3.
3. The *d-d* transition band has a much higher absorption coefficient (ε) than the LMCT band.
4. OH^- is more likely to form insoluble salts with 3+ transition metal ions than S^{2-}.
5. O^{2-} ion has a larger radius than Na^+ ion.
6. Substitution reaction with $\Delta H^{\neq} = 80KJ/mol$, and $\Delta S^{\neq} = -13$ e.u. indicates associative mechanism.
7. The active center of the deoxy form hemoglobin contains a five-coordinated-ironprophyrin with low spin Fe(III) metal center.
8. Tetragonally elongated (z-out) O_h ligand field lowers the d_{xz} and d_{yz} orbitals in energy.
9. Circular dichroism, CD, is defined by $\varepsilon_l - \varepsilon_r$, where ε_l and ε_r are the molar absorption coefficients for left and right circularly polarized light.
10. Olefins are weaker field ligands than NH_3.

III. 問答題 (共 20 分)

1. (15 分) Draw structure for the following complexes:
(1) $Al_2(CH_3)_6$ (2) $[Bi_5]^{3+}$ (3)all isomers of *mer*-$Fe(H)_2(PPh_3)(CO)_3$
2. (5 分) Draw a diagram that illustrates the bonding and back-bonding interactions for a metal-H_2 complex.

PART I (two points for each problem) 單選題；答錯不倒扣分數

1. The potential function associates to the vibration of a diatomic molecule can be adequately described by

(a). Harmonic oscillator
(b). Morse function
(c). Coulombic type potential
(d). Lenard-Jones type potential
(e). None of above is correct

2. According to Born-Oppenheimer approximation, which property of HCl and DCl is the same?

(a) dissociation energy
(b). ground state vibration energy
(c). vibration force constant
(d). reduced mass
(e). All of the above are different

3. Which of the following molecules has the largest rotation constant?

(a) H_2
(b). HCl
(c). N_2
(d). HF
(e). All the same

4. The rotation constant of a diatomic molecule is useful for the determination of

(a) vibration frequency
(b). bond length
(c). force constant
(d). dissociation energy
(e). None of above is correct

5. The quantum mechanical expression of any angular momentum operator

(a) depends on the mass of the particle
(b). has no distance dependence
(c). has no associate eigen function
(d). always has eigen value 1/2
(e). none of above is correct

6. If three operators $\hat{A}, \hat{B}$ and $\hat{C}$ has the following relations:

$$\left[\hat{A},\hat{B}\right]=0, \qquad \left[\hat{B},\hat{C}\right]=\hat{A}$$

(a). $\hat{A}$ and $\hat{C}$ must commute
(b). $\hat{B}$ and $\hat{C}$ has common eigen values
(c). One can not measure the physical properties associate to $\hat{A}$ and $\hat{B}$ simultaneously
(d). $\left[\hat{A},\hat{C}\right]=-\hat{B}$
(e). None of above is correct

7. In which of the following systems a free particle may have the largest degeneracy in its energy levels?

(a). triangle box
(b). circular box
(c). ellipse box
(d). square box
(e). all the same

8. Which of the following types of energy has the largest magnitude?

(a). rotational energy
(b). translational energy
(c). electronic energy
(d). vibrational energy
(e). zero-point energy

9. Which of the following effects can be explained by Franck Condon principle?

(a) overtone in infarad spectrum
(b) combination mode in vibrational spectrum
(c) largest intensity of fundamental
(d) largest intensity of overtone
(e) None of above

10. Which theory or postulation links classical property to quantum mechanical property?

(a). de Broglie theory
(b). Heisenberg uncertainty principle
(c). Bohr H-atom model
(d). Einstein photo-electric effect
(e). None of above

11. Which factor is important to calculate collision frequency of gas molecules?

(a). density of the gas
(b). diamter of the molecule
(c). average velocity of the molecule
(d). temperatue
(e). All of above are important

12. The electron in H atom has orbital angular momentum $\vec{L}$ and spin angular momentum $\vec{S}$. In quantum mechanics, the associate operators are $\hat{L}$ and $\hat{S}$ respectively. Which of the following statements is incorrect?

(a). $\hat{L}^2$ and $\hat{S}^2$ are quantized

(b). $|\vec{L}| = |\vec{S}|$

(c). the z-components of $\vec{L}$ are quantized

(d). the z-components of $(\vec{L} + \vec{S})$ are quantized

(e). $[\hat{L}^2, \hat{L}_z] = [\hat{S}^2, \hat{S}_z]$

13. Harmonic oscillator is an useful model to describe the vibration of diatomic molecules. Which of the following statements about the model is incorrect?

(a). the average kinetic energy equals to the average potential energy
(b). the dissociation energy of a diatomic molecule can not be estimated from this model
(c). the energy levels are equally spaced
(d). the wave functions of all vibration states have same symmetry properties.
(e). the vibration frequency is related to the reduced mass of the molecule

14. For an ideal gas, which is correct?

6-3

(a). $C_P - C_V = 3R/2$

(b). $\Delta U = 0$ for an isothermal expansion process

(c). $Q = 0$ for an isothermal expansion process

(d). ΔS is independent of temperature for isothermal expansion processes

(e). $\Delta G < 0$ for an isothermal compression process

15. Two operators $\hat{A} = x$, $\hat{B} = x\dfrac{d}{dx}$, then

(a). $\hat{A}$ and $\hat{B}$ commute

(b). $\left[\hat{A}, \hat{B}\right] = x^2$

(c). $\left[\hat{B}, \hat{A}\right] = x$

(d). $\left[\hat{A}^2, \hat{B}\right] = -x^2$

(e). none of above is correct

16. Which description of an irreversible reaction is right?

(a) $d\mathrm{S} = d\mathrm{q} / \mathrm{T}$

(b) $d\mathrm{G} = d\mathrm{H} - \mathrm{T}d\mathrm{S}$

(c) $d\mathrm{q} < \mathrm{T}d\mathrm{S}$

(d) $d\mathrm{w} \leq d\mathrm{H}$

(e) none of above

17. Why entropy is measured by heat?

(a) Because heat is not a state function.

(b) Because entropy is a function of temperature.

(c) Because entropy is heat energy.

(d) Because heat is thermal disorder motions of atoms.

(e) None of above is right.

18. What's the physical meaning of fugacity of a material?

(a) $\left(\frac{\partial U}{\partial V}\right)_T$.

(b) Surface tension.

(c) effective pressure.

(d) a fugitive.

(e) slope of reaction heat.

19. The measured Joul-Thomson coefficient for CO_2 at 300 K and 1 atom is 1.1045.

(a). the gas is warming on expansion

(b). the gas is cooling on compression

(c). one can liquefy the gas by reducing the pressure

(d). the gas is ideal gas

(e). none of above is correct

20. Which of the following differential is incorrect?

(a). $dU = \left(\dfrac{\partial U}{\partial S}\right)_V dS + \left(\dfrac{\partial U}{\partial V}\right)_S dV$

(b). $dH = \left(\dfrac{\partial H}{\partial P}\right)_S dP + \left(\dfrac{\partial H}{\partial S}\right)_P dS$

(c). $dG = \left(\dfrac{\partial G}{\partial T}\right)_V dT + \left(\dfrac{\partial G}{\partial V}\right)_T dV$

(d). $dA = \left(\dfrac{\partial A}{\partial V}\right)_T dT + \left(\dfrac{\partial A}{\partial T}\right)_V dV$

(e). $dV = \left(\dfrac{\partial V}{\partial T}\right)_P dT + \left(\dfrac{\partial V}{\partial P}\right)_T dP$

PART II (4 points for each problem)

21. For an isothermal expansion of one mole of ideal gas form V_1 to V_2, we found that the entropy is increased by 11.48 $J \cdot K^{-1}$, then $V_1 / V_2 =$? (given gas constant $R = 8.28\ J \cdot K^{-1}$)

(a). 0.6
(b). 0.333
(c). 0.5
(d). 0.25
(e). 0.693

22. The heat of reaction may be obtained by the slop of which plot?

(a). logrithm of rate coefficient v.s inverse of temperature
(b). logrithm of the concentration of the product v.s reaction time
(c). logrithm of equilibrium constant v.s inverse of temperature
(d). logrithm of reaction rate v.s the concentraion of the reactant
(e). none is correct

23. For a system with the two competing elementary reactions

$A \xrightarrow{k_1} B$ and $A \xrightarrow{k_2} B$

The activation energies of two reactions are E_1 and E_2, then the overall activation energy of the system is:

(a). $E_1 + E_2$
(b). $\ell n(E_1 + E_2)$
(c). $(k_1 e^{-E_1/kT} + k_2 e^{-E_2/kT})/(k_1 + k_2)$
(d). $(k_1 E_1 + k_2 E_2)/(k_1 + k_2)$
(e). none is correct

24. Giving a free particle in a one-dimensional box ($0 \le x \le a$), which of the following statement is incorrect?

(a). Move the box to $a \le x \le 2a$ results different energy levels of the system
(b). Shrink the box to $0 \le x \le a/2$ has no effect on the wave function of the particle
(c). Enlarge the box to $0 \le x \le 2a$ will reduce the probability of finding the particle in the range $a/2 \le x \le a$
(d). Enlarge the box to $0 \le x \le 2a$ has no effect on the averaged value of the momentum of the particle.
(e). The symmetry properties of the wave functions are independent on the dimension of the box.

25. The ground state wave function of hydrogen atom is $\psi = \frac{1}{\pi^{1/2}} \left(\frac{1}{a_0} \right)^{3/2} e^{-r/a_0}$,

where $a_0 = 0.529A$. Which statement is correct?

(a). The probability of finding the electron within radial distance b can be calculated by $P = \int_0^b |\psi|^2 dr$

(b). The average radial distance can be evaluated by $\langle r \rangle = \int_0^\infty \psi^2 r^3 dr$

(c). The most probable radial distance of the electron can be calculated by maximizing the function $F(r) = \psi^2 r^3$

(d). The averaged value of $1/r^2$ is $2/a_0^2$

(e). None of above is correct

26. The empirical rate law for the reaction $H_2(g) + Br_2(g) \rightarrow 2HBr(g)$ is

$$\frac{d[HBr]}{dt} = \frac{k[H_2][Br_2]^{3/2}}{[Br_2] + k'[HBr]}$$

Where k and k' are rate constants respectively. Which of the following processes may be useful to determine k?

(a). Decrease concentration of H_2

(b) Increase temperature

(c) Eliminate $[HBr]$ immediately after it is formed

(d) Use large excess concentration of Br_2

(e) None of above is correct

27. The half life of the first order reaction $C_2H_6 \rightarrow 2CH_3$ is 21.6 min. Predict the reaction time when 3/4 of the initial C_2H_6 is converted to CH_3

(a). 10.8 min

(b). 8.98 min

(c). 43.3 min

(d). 37.6 min

(e). None is correct

28. The distribution function of gas molecular system is

$$F(c) = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp(-mc^2/2kT) \cdot 4\pi c^2$$

In which m and c are the mass and speed of the molecule, k and T are Boltzmann constnat and absolute temperature respectively. Which of the following statements is correct ?

(a). average speed can be calculated by $\int_{-\infty}^{\infty} cF(c)dc$

(b) The most probable value of maximum speed can be calculated by setting $dF(c)/dc = 0$

(c). The total area under the distribution curve $F(c)$ vs. c is one.

(d). The maximum speed shifts to small value when temperature increases

(e). All answers are correct

29. The three wave functions ψ_{nlm} of H atom for states $n = 2$, $\ell = 1$ are

$\psi_{210} = \frac{1}{\sqrt{32\pi}} re^{-r/2} \cos\theta$, $\psi_{21\pm1} = \frac{1}{\sqrt{64\pi}} re^{-r/2} \sin\theta e^{\pm i\phi}$, where r, θ and ϕ are spherical polar coordinates.

(a). the energies of these states are different

(b). $\psi_{2px} = \psi_{210}$

(c). $\psi_{2p_y} = \frac{1}{\sqrt{2}}(\psi_{211} - \psi_{21-1})$

(d). Apply magnetic field on H atom system will change the energy of ψ_{210} but not $\psi_{21\pm1}$

(e). None is correct

30. Which of the following functions may be used to obtain the approximate ground state energy of a particle within a box $(0 \le x \le 1)$.

(a). $\phi(x) = (1-x)(1+x)$ (b). $\phi(x) = \sin x$

(c). $\phi(x) = \cos(x/2)$ (d). $\phi(x) = x - x^2$

(e). $\phi(x) = e^{-x^2}$

31. The Infarad spectroscopy determines the fundamental frequency of a diatomic molecule is 1200 cm^{-1} and the rotation constant is 20 cm^{-1}. Which of the following is approximately the transition frequency from $(n, J) = (1,4)$ to $(n', J') = (2,3)$? Where n and J are vibration and rotation quantum numbers respectively.

(a). 1220 cm^{-1} (b). 1180 cm^{-1}

(c). 640 cm^{-1} (d). 1160 cm^{-1}

(e). None of above is correct

32. The equilibrium constant for a specific reaction is K=10.0 at temperature 200K, and K=100.0 at 400K. What is the equilibrium constant at 800K?

(a) 1000.0 (b) 100000.0

(c) 316.23 (d) 3162.3

(e) 177.83

33. If the wave function of a particle in a box $(-1 \le x \le 1)$ is $\phi(x) = 1 - x^2$, then, the average value of x^2 is

(a). 0 (b). 16/105

(c). 1/35 (d). 1/30

(e). none is correct

34. The entropy change of mixing 2 moles of N_2 and 4 moles of Ar at 273 K is approximately equal to ? (giving R is gas constant)

(a). 0.636R (b). 6.931R

(c). 0.514R (d). -1.828R

(e). none is correct

35. The overall C_p of reaction $H_2O(g) \rightarrow H_2(g) + \frac{1}{2}O_2(g)$ is $C_p = 9.83 J \cdot K^{-1} \cdot mol^{-1}$ and the reaction enthalpy is 241.75 kJ at 291.15 K. The reaction enethalpy at 298 K is

(a). 253.1 kJ (b). 241.82 kJ

(c). 244.58 kJ (d). 282.33 kJ

(e). None is correct

1. (a) What is reversed phase chromatography. (b) If a mixture of two compounds containing n-hexane and n-hexanol will be separated from this column, please compare the retention time for them to come out from the column. (8%)
2. (a) Discuss the effect of pH on the intensity of fluorescence and explain the reason? You can give an example to explain it as detailed as possible if you have difficulty to explain. (b) Discuss the temperature effect on the intensity of fluorescence and explain the reason? (8%)
3. Predict the order of chemical shift parameters for CHX_3 (where X=F, Cl, Br and I). Please also explain the reason based on the electronegativity. (8%)
4. (a) What is the internal standard method? Please describe the principle and also discuss the application for this method. You can give an example to explain it as detailed as possible if you have difficulty to explain. (b) What is solid phase microextraction (SPME)? Please describe the principle and also discuss the application for this technique. (8%)
5. Calculate the molar solubility of $Mg(OH)_2$ in water. Ksp = 7.1×10^{-12} (8%).
6. (a) Define RSD (b) Define LOD. You must first write down the full name in English for these terms and then give detailed description for the definition. You can give an example to explain its definition as detailed as possible if you have difficulty to explain. (8 %)
7. Select the following ionization method(s) of mass spectrometry (MS) that can be powerful technique(s) for the study of bacteria via commercial MS instrument(s)? FI (Field Ionization), MALDI (matrix assisted laser desorption/ionization), ESI (Electrospray Ionization), EI (Electronic Ionization), CI (Chemical Ionization), APCI (atmospheric pressure chemical ionization), FD (Field Desorption), FAB (fast atom bombardment), inductively coupled plasma (ICP), APPI (atmospheric pressure photoionization), Glow discharge, plasma desorption. (8%)
8. One graduate student synthesized some nanoparticles and then he wanted to select suitable instruments to analyze his nanoparticles. Discuss all instruments listed below in terms of their capability in identification or determination the sizes of the nanoparticles. According to your best knowledge, discuss how he can apply all these instruments to characterize nanoparticles and also describe their functions for nanoparticle analysis. Please describe as detailed as possible for each instrument. You can also give some examples for what type of nanoparticles can be analyzed. (1) UV/Vis (2) FT-IR (3) TEM (4) SEM (5) Fluorospectrometer (Flu) (6)AFM (7) MALDI-TOF-MS (8) ESI-MS. (8%, 1 point for each instrument)
9. Can you indicate feasible schemes or methods that might include using sample pretreatment techniques, separation methods and then can be successfully

detected by using the analytical instrument(s). Please describe the reasons or the principles for your proposed methods for the following analysis (1) benzene in water (2) lead in blood (3) caffeine from tea.(6%, 2 points for each item)

10. Discuss all instruments listed below in terms of their capability in identification purposes or functions for compound analysis. Please also give some real examples for compounds to be analyzed by each instrument. You must describe as detailed as possible to demonstrate your understanding for how to use (apply) these instruments in general purposes. (1) UV/Vis (2) IR (3) NMR (4) ICP-AES (5) Fluorospectrometer (Flu) (6) AAS (7) QCM (8) MALDI-MS (9) GC/MS (10) CE (11) HPLC. (22%, 2 points for each instrument)
11. Calculate the energy of a photon with a wavelength of 8.00 μm (in the air).(8%)

Important Physical Constants

Constant	Symbol	Value
Speed of light (*vacuo*)	c	2.99792×10^{8} ms^{-1}
Planck constant	h	6.62608×10^{-34} J s
Avogadro number	N	6.022137×10^{23} particles mol^{-1}
Faraday constant	F	96485.31 C mol^{-1}
Gas constant	R	$8.31451 \times$ J K^{-1} mol^{-1}
		0.0820578 L atm K^{-1} mol^{-1}
Boltzmann constant	k	1.38066×10^{-23} J K^{-1}
Rest mass of the electron	m_e	9.10939×10^{-31} kg
Electronic charge	e	$-1.602177 \times 10^{-19}$ C

Energy Conversion Factors

	Joules	Ergs	Calories	Liter Atmosphere	Electron Volts
1 joule =	1	10^{7}	2.3901×10^{-1}	9.8687×10^{-3}	6.2418×10^{18}
1 erg =	10^{-7}	1	2.3901×10^{-8}	9.8687×10^{-10}	6.2418×10^{11}
1 calorie =	4.1840	4.1840×10^{7}	1	4.1291×10^{-2}	2.6116×10^{19}
1 liter atmosphere =	1.0133×10^{2}	1.0133×10^{9}	24.218	1	6.3248×10^{20}
1 electron volt =	1.6021×10^{-19}	1.6021×10^{-12}	3.8291×10^{-20}	1.5811×10^{-21}	1