

ENTRANCE EXAMINATION FOR ADMISSION, MAY 2011.

M.Phil./Ph.D. (CHEMISTRY)

COURSE CODE : 244/107

Register Number :

*Signature of the Invigilator
(with date)*

COURSE CODE : 244/107

Time : 2 Hours

Max : 400 Marks

Instructions to Candidates :

1. Write your Register Number within the box provided on the top of this page and fill in the page 1 of the answer sheet using pen.
2. Do not write your name anywhere in this booklet or answer sheet. Violation of this entails disqualification.
3. Read each question carefully and shade the relevant answer (A) or (B) or (C) or (D) in the relevant box of the ANSWER SHEET using HB pencil.
4. Avoid blind guessing. A wrong answer will fetch you -1 mark and the correct answer will fetch 4 marks.
5. Do not write anything in the question paper. Use the white sheets attached at the end for rough works.
6. Do not open the question paper until the start signal is given.
7. Do not attempt to answer after stop signal is given. Any such attempt will disqualify your candidature.
8. On stop signal, keep the question paper and the answer sheet on your table and wait for the invigilator to collect them.
9. Use of Calculators, Tables, etc. are prohibited.

- The strongest Jahn-Teller distortion is observed for
 - Cr (II)
 - Mn (IV)
 - Ni (III)
 - Cu (II)
- The biological function of hemerythrin is
 - oxygen transport
 - photosynthesis
 - metal storage
 - electron transfer
- The colour of vanadium pentoxide is due to
 - d-d transition
 - charge transfer transition
 - point defect
 - non-stoichiometry
- In X-ray, the position of following atom can not be estimated accurately
 - hydrogen
 - lithium
 - helium
 - chlorine
- The number of metal-metal bonds in $[(C_5H_5)Fe(CO)_2]_2$ is
 - zero
 - one
 - two
 - three
- The bond orders of O_2 , O_2^+ , O_2^- and O_2^{2-} will be in the order of
 - $O_2 > O_2^+ > O_2^- > O_2^{2-}$
 - $O_2^+ > O_2 > O_2^- > O_2^{2-}$
 - $O_2^{2-} > O_2^- > O_2^+ > O_2$
 - $O_2^{2-} > O_2^- > O_2 > O_2^+$
- The catalyst used in the conversion of ethylene to acetaldehyde using Wacker process is
 - $HCo(CO)_4$
 - $[PdCl_4]^{2-}$
 - V_2O_5
 - $TiCl_4$ and $Al(C_2H_5)_3$
- The metal present in cytochrome is
 - copper
 - cobalt
 - iron
 - magnesium
- The ordering of the d-orbital energies in an octahedral complex on tetragonal elongation is expected to be
 - $d_{xy} > d_{yz}, d_{xz} > dz^2 > dx^2-y^2$
 - $dx^2-y^2 < dz^2 < d_{xy} > d_{yz}, d_{xz}$
 - $dx^2-y^2 > dz^2 > d_{xy} > d_{yz}, d_{xz}$
 - $dx^2-y^2 > d_{xy} > dz^2 > d_{yz}, d_{xz}$

10. The crystal field stabilization energy for an octahedral complex with electronic configuration t_{2g}^3, e_g^2 is
 (A) 0 (B) 0.4Δ (C) 1.2Δ (D) 1.6Δ
11. The inert is ascribed to the group VIII A elements is due to
 (A) very high electronegativity (B) very high ionization energy
 (C) very high electron affinity (D) very high
12. The ^1H NMR spectrum of HD consists of a
 (A) singlet (B) 1:1 doublet
 (C) 1:1:1 triplet (D) 1:2:1 triplet
13. Which one of the following statements about diborane is **not correct**?
 (A) It has one two-center two-electron B - B bond.
 (B) Diborane is highly air-sensitive when it is not extremely pure.
 (C) It has two three-center two-electron B - H - B bonds.
 (D) It acts as a Lewis acid.
14. The metal ion that is expected to shift the C_1 methylene group in heptanol from 2 to 10 ppm in ^1H NMR is
 (A) Eu(III) (B) Tl(III) (C) Al(III) (D) Sc(III)
15. The homogeneous catalyst used in the hydroformylation is based on
 (A) cobalt (B) chromium (C) titanium (D) vanadium
16. Among the following, the isoelectronic and isostructural pair is
 (A) CO_2 and SO_2 (B) SO_3 and SeO_3
 (C) NO^{2+} and TeO_2 (D) SiO_4^{4-} and PO_4^{3-}
17. A physical method that can be used to identify the compounds, $[\text{NiCl}_2(\text{PPh}_3)_2]$ and $[\text{PdCl}_2(\text{PPh}_3)_2]$ unambiguously is
 (A) HPLC (B) EXAFS
 (C) Magnetic susceptibility (D) Mossbauer spectroscopy
18. The correct statement about the Cu-N bond distances in $[\text{Cu}(\text{NH}_3)_6]^{2+}$ is
 (A) all the bond distances are equal
 (B) the axial bonds are longer than the equatorial ones
 (C) the equatorial bonds are longer than the axial ones
 (D) all the bond distances are unequal

19. The reaction of

$$[\text{Co}(\text{H}_2\text{O})_5\text{Cl}]^{2+} + [\text{Cr}(\text{H}_2\text{O})_6]^{2+} \rightarrow [\text{Co}(\text{H}_2\text{O})_6]^{2+} + [\text{Cr}(\text{H}_2\text{O})_5\text{Cl}]^{2+}$$
occurs through the following mechanism
- (A) $\text{S}_{\text{N}}1$ (B) isomerisation
(C) inner sphere (D) outer sphere
20. 2.5 g of an iron compound upon suitable treatment yielded 0.391 g of iron(III) oxide (atomic weight of Fe: 55.847, O: 15.994). The percentage of iron in the compound is,
(A) 10.94 (B) 12.15 (C) 11.31 (D) 9.11
21. In EPR spectroscopy, the selection rule is
(A) nuclear spin changes, while electron spin does not change
(B) electron spin changes, while nuclear spin does not
(C) both electron and nuclear spin change
(D) both electron spin and nuclear spin do not change
22. Treatment of $\text{W}(\text{CO})_6$ with one equivalent of $\text{Na}(\text{C}_5\text{H}_5)$ in THF solution gives the ionic compound **M**. Reaction of **M** with glacial acetic acid results in product **N**. The ^1H NMR spectrum of **N** displays two singlets of relative intensity 5:1. The compounds **M** and **N**, respectively, are
(A) $[(\text{C}_5\text{H}_5)\text{W}(\text{CO})_3]\text{Na}$ and $[(\text{C}_5\text{H}_5)\text{W}(\text{CO})_3\text{H}]$
(B) $[(\text{C}_5\text{H}_5)\text{W}(\text{CO})_4]\text{Na}$ and $[(\text{C}_5\text{H}_5)\text{W}(\text{CO})_4\text{H}]$
(C) $[(\text{C}_5\text{H}_5)\text{W}(\text{CO})_3]\text{Na}$ and $[(\text{C}_5\text{H}_5)\text{W}(\text{CO})_4\text{H}]$
(D) $[(\text{C}_5\text{H}_5)\text{W}(\text{CO})_4]\text{Na}$ and $[(\text{C}_5\text{H}_5)\text{W}(\text{CO})_3\text{H}]$
23. Triphosphazene is prepared by reacting **X** and **Y** in equimolar ratio at 120-150° C using appropriate solvents. The reactants **X** and **Y**, respectively, are
(A) PCl_3 and NH_3 (B) PCl_5 and NH_3
(C) PCl_5 and NH_4Cl (D) PCl_3 and NH_4Cl
24. The total number of isomers of $[\text{Co}(\text{en})_2\text{Cl}_2]$ is
(A) four (B) three (C) six (D) five
25. The structures of the complexes $[\text{Cu}(\text{NH}_3)_4](\text{ClO}_4)_2$ and $[\text{Cu}(\text{NH}_3)_4](\text{ClO}_4)$ in solution respectively are
(A) square planar and tetrahedral (B) octahedral and square pyramidal
(C) octahedral and trigonal bipyramidal (D) tetrahedral and square planar

26. The number of M-M bonds in $\text{Ir}_4(\text{CO})_{12}$ are
 (A) four (B) six (C) eight (D) zero
27. In biological systems, the metal ions involved in electron transport are
 (A) Na^+ and K^+ (B) Zn^{2+} and Mg^{2+}
 (C) Ca^{2+} and Mg^{2+} (D) Cu^{2+} and Fe^{3+}
28. If ClF_3 were to be stereochemically rigid, its ^{19}F NMR spectrum ($I = \frac{1}{2}$ for ^{19}F) would be (assume that Cl is not NMR active)
 (A) a doublet and a triplet (B) a singlet
 (C) a doublet and a singlet (D) two singlets
29. In the complex, $[\text{Ni}_2(\eta^5\text{-Cp})_2(\text{CO})_2]$, the IR stretching frequency appears at 1857 cm^{-1} (strong) and 1897 cm^{-1} (weak). The valence electron count and the nature of the M-CO bond respectively are
 (A) 16 e^- , bridging (B) 17 e^- , bridging
 (C) 18 e^- , terminal (D) 18 e^- , bridging
30. The reaction of PCl_3 with methanol in presence of triethylamine affords compound X. EI mass spectrum of X shows a parent ion peak at $m/z = 124$. Microanalysis of X shows that it contains C, H, O and P. The ^1H NMR spectrum of X shows a doublet at 4.0 ppm ($I = \frac{1}{2}$ for ^{31}P). The compound X is
 (A) $(\text{CH}_3\text{O})_3\text{P}$ (B) $(\text{CH}_3\text{O})_2\text{P}(\text{O})$
 (C) $(\text{CH}_3\text{O})_2\text{P}(\text{O})(\text{OH})$ (D) $(\text{CH}_3\text{O})_3\text{PH}$
31. The number of carbon-13 signals expected for 2,6-dihydroxynaphthalene in its ^1H decoupled ^{13}C NMR spectrum is
 (A) three (B) four (C) five (D) six
32. The reaction of indole with acetic anhydride leads to
 (A) 4-acetylindole (B) 1-acetylindole
 (C) 2-acetylindole (D) 3-acetylindole
33. The characteristic absorption band (cm^{-1}) for butanal and butyronitrile respectively are
 (A) 1725 and 1795 (B) 1680 and 2240
 (C) 1795 and 2240 (D) 1725 and 2240

34. Which among the following exhibit characteristics of aromatic compounds?
i. Cyclopentadiene; ii. Ferrocene; iii. Pentadienyl cation; iv. Pyrrole
(A) i and ii (B) ii and iii (C) ii and iv (D) iii and iv
35. The orientation of two methyl groups in the stable configuration of *cis*-1,2-dimethylcyclohexane are
(A) equatorial and equatorial (B) equatorial and axial
(C) axial and axial (D) axial and pseudo-equatorial
36. The reaction of cyclohexanone sequentially with i. pyrrole and ii. chlorine gas at -78°C leads to
(A) 4-chlorocyclohexanone (B) 2,4-dichlorocyclohexanone
(C) 2-chlorocyclohexanone (D) 2,6-dichlorocyclohexanone
37. The reaction of 1-hexyne with methyl magnesium bromide yields
(A) 1-hexynylmagnesium bromide and methane
(B) 2-hexynylmagnesium bromide and ethane
(C) 1-octyne
(D) 3-octyne
38. The reaction of hexanoic acid with excess of methyl lithium followed by hydrolysis leads to
(A) heptanal (B) 2-heptanone (C) 2-octanone (D) 3-octanone
39. The reaction of cyclohexene with N-bromosuccinimide in methanol yields
(A) 3-bromocyclohexene
(B) 4-bromocyclohexene
(C) *trans*-1-bromo-2-methoxycyclohexane
(D) *cis*-1-bromo-2-methoxycyclohexane
40. The stereochemistry of ring junction in the product formed in the cycloaddition of butadiene with 1,4-benzoquinone
(A) *cis* (B) *trans* (C) *syn* (D) *anti*
41. The acid catalyzed rearrangement of cyclopentanone oxime to corresponding lactam is an example for
(A) Pinacol-pinacolone rearrangement (B) Beckman Rearrangement
(C) Cope Rearrangement (D) Claisen Rearrangement

42. The reaction of cyclohexenone with i. ethane dithiol, $\text{BF}_3 \cdot \text{Et}_2\text{O}$, ii. Raney Ni is expected to provide
- (A) cyclohexane (B) cyclohexene
(C) cyclohexanone (D) cyclohexanol
43. The reaction of 3,5,5-trimethyl-2-cyclohexene-1-one with i. para-tolunesulfonylhydrazine, ii. methyl lithium is expected to provide
- (A) 1,3,3-trimethyl-1-cyclohexene (B) 3,3,5-trimethyl-1-cyclohexene
(C) 2,4,4-trimethyl-1-cyclohexene (D) 2,6,6-trimethyl-1,3-cyclohexadiene
44. The reaction of benzonitrile with ethyl magnesium iodide provides
- (A) benzaldehyde (B) acetophenone
(C) propiophenone (D) phenyl acetaldehyde
45. A five carbon aldose **A** on reduction with sodium borohydride gives an optically inactive product. The aldose **A** on one carbon homologation using Kiliani synthesis results in D-glucose and D-idose. The aldose **A** is
- (A) D-xylose (B) D-lyxose (C) D-arabinose (D) D-ribose
46. Reaction of phenyl azide with dimethyl acetylene dicarboxylate gives
- (A) imidazole (B) pyrrole (C) triazole (D) triazine
47. When 1-methyl-3-(vinyl-oxo)-1-cyclohexene is heated to 200°C , the product formed is
- (A) (2-methyl-2-cyclohexenyl)acetic acid
(B) methyl 2-(1-methyl-2-cyclohexenyl)acetate
(C) 2-(1-methyl-2-cyclohexenyl)acetaldehyde
(D) 2-(1-methyl-3-cyclohexenyl)acetaldehyde
48. The base mediated condensation of dibenzylketone with benzil yields
- (A) 2,3,4,5-tetraphenylcyclopentadienone
(B) 2,3,4-triphenylcyclopentadienone
(C) 2,3-diphenylcyclopentadienone
(D) 2,5-diphenylcyclopentadienone

49. Acetone is condensed with cyclopentadiene in presence of sodium hydride. The product formed is
- (A) dicyclopentadiene
 (B) dimethylfulvene
 (C) morpholine oxide
 (D) 2,2-dimethyl-2,2a,5,5a-tetrahydrocyclopenta[*b*]oxete
50. The major product obtained in the reaction between 2-phenylacetonitrile $\text{HNO}_3/\text{H}_2\text{SO}_4$ would be
- (A) phenyl acetic acid
 (B) 2-(2-nitrophenyl)acetonitrile
 (C) 2-(3-nitrophenyl)acetonitrile
 (D) 2-(4-nitrophenyl)acetonitrile
51. The reaction of an alkene with ozone followed by treatment with hydrogen peroxide resulted in two moles of butanoic acid. The alkene is
- (A) 1-butene
 (B) 2-hexene
 (C) 4-octene
 (D) 6-dodecene
52. An organic compound exhibits molecular ion peak (also base peak) at m/z 91 in its mass spectrum. The ^1H NMR spectrum shows signals at 3.85 (s, 3H), 7.0 (d, $J = 7.8$ Hz, 2H), 7.85 (d, $J = 7.8$ Hz, 2H), 9.9 (s, 1H). The compound is
- (A) 2-hydroxy acetophenone
 (B) 4-hydroxy acetophenone
 (C) 2-methoxy benzaldehyde
 (D) 4-methoxy benzaldehyde
53. The reaction of 3-hexyne with sodium/ammonia is expected to yield
- (A) *E*-3-hexene
 (B) *Z*-3-hexene
 (C) Hexane
 (D) Dodecane
54. An organic compound of molecular formula $\text{C}_8\text{H}_{10}\text{O}_2$ exhibits base peak at 94. Its IR spectrum shows a broad band at 3300 cm^{-1} . The ^1H NMR spectrum shows signals at δ 2.4 (1H, washable with D_2O), 3.9 (m, 2H), 4.2 (t, 2H), 6.9 (m, 3H), 7.4 (t, 2H). The compound could be
- (A) 4-(2-hydroxyethyl)phenol
 (B) 2-(2-hydroxyethyl)phenol
 (C) 2-(1-hydroxyethyl)phenol
 (D) 2-phenoxy-1-ethanol
55. The characteristic IR absorption band (cm^{-1}) for ethyl acetate and butyrolactone respectively are
- (A) 1775 and 1735
 (B) 1680 and 1735
 (C) 1735 and 1775
 (D) 1735 and 2240

56. Rearrangement of pinacol to pinacolone under acidic conditions goes through
 (A) carbanion (B) carbocation
 (C) carbene (D) free radical
57. A neutral organic compound of molecular formula $C_8H_8O_2$ showed prominent band at 1764 cm^{-1} . The mass spectrum of this compound showed base peak at m/z 94. The 1H NMR spectrum showed a singlet at δ 2.4 ppm. The compound could be
 (A) phenyl acetic acid (B) methyl benzoate
 (C) 4-methylbenzoic acid (D) phenyl acetate
58. Rearrangement of 2-chlorocyclohexanone to methyl cyclopentane carboxylic acid with sodium methoxide goes through
 (A) carbanion (B) carbocation
 (C) carbene (D) free radical
59. The biosynthetic precursors for the alkaloid reserpine are
 (A) tyrosine and pinene (B) tryptophan and secologanin
 (C) lysine and geraniol (D) phenyl alanine and camphor
60. An organic compound of MF $C_7H_{14}O$ answers Tollen's test. Prominent bands in IR spectrum are 2716 and 1727 cm^{-1} . The ^{13}C NMR spectrum of the compound shows seven distinct signals. The compound could be
 (A) 2-methylhexanal (B) 5-methylhexanal
 (C) heptanal (D) 2-heptanone
61. Which of the following pairs of physical quantities commute?
 (A) x and p ; x is position vector and p is the momentum
 (B) v and t ; v is frequency and t is the time,
 (C) K and λ ; K is the wave vector and λ is the de Broglie wavelength
 (D) L and ϕ ; L is the angular momentum and ϕ azimuthal angle
62. The numbers of radial nodes of 3d orbital is
 (A) 3 (B) 2 (C) 1 (D) 0
63. If ψ_a and ψ_b are the atomic wave functions of the two hydrogen atoms, then for the bonding sigma-bonding orbital of hydrogen molecule, the increase in the electronic probability density between the two hydrogen atoms is
 (A) $\psi_a \psi_b$ (B) $2\psi_a \psi_b$ (C) $-\psi_a \psi_b$ (D) $-2\psi_a \psi_b$

64. The numbers of classes in the C_{3v} point group symmetry is
 (A) 1 (B) 2 (C) 3 (D) 4
65. The general formula of a spinel is
 (A) AB_2O_4 (B) $A_2B_2O_3$ (C) A_2BO_4 (D) AB_3O_4
66. Which of the following is not a thermoelectric effect?
 (A) Thomson effect (B) Seebeck effect
 (C) Peltier effect (D) Meissner effect
67. The mean square average distance, $\langle x^2 \rangle$, of a diffusing species after time t is
 (A) $\langle x^2 \rangle = 2Dt$ (B) $\langle x^2 \rangle = Dt$ (C) $\langle x^2 \rangle = 2Dt^2$ (D) $\langle x^2 \rangle = 3Dt$
68. The number of variables in phase space is
 (A) 3 (B) 4 (C) 5 (D) 6
69. The total number of hyperfine lines in an isotropic EPR spectrum of V^{4+} ion is
 (A) 2 (B) 4 (C) 6 (D) 8
70. Which of the following plane is not parallel to the z -axis?
 (A) (001) (B) (110) (C) (100) (D) (010)
71. Which of the following is true for melting?
 (A) exothermic process (B) endothermic process
 (C) irreversible process (D) none of the above
72. In Bragg formula $n\lambda = 2d \sin \theta$, the possible value(s) on the order reflection, n , is given by
 (A) 1 only (B) 2 only
 (C) 3 only (D) all values as above
73. The standard reduction potentials of Mg/Mg^{2+} is -2.360 V, and Cu/Cu^{2+} is 0.337 V. The standard cell emf for the reaction, $Mg + Cu^{2+} \rightarrow Mg^{2+} + Cu$, is
 (A) 2.697 V (B) -2.697 V (C) -2.023 V (D) 2.02 V
74. Which of the following is not a Van der Waal force?
 (A) Dipole-dipole interaction (B) London dispersion force
 (C) Dipole induced-dipole force (D) Hydrogen bonding

75. In a two component solid-solid phase diagram, the degrees of freedom at the eutectic point is/are
(A) 3 (B) 2
(C) 1 (D) 0
76. The SI unit of viscosity is
(A) $\text{Kg S}^{-1}\text{m}^{-1}$ (B) Kg S m^{-1}
(C) $\text{Kg}^{-1} \text{S}^{-1}\text{m}^{-1}$ (D) $\text{Kg}^{-1}\text{S}^{-1}\text{m}$
77. The order of the reaction $\text{H}_2 + \text{Br}_2 = 2\text{HBr}$ is
(A) first order (B) second order
(C) zeroth order (D) none of the above
78. The number of normal modes of vibration in H_2S molecule is
(A) 4 (B) 2
(C) 3 (D) 1
79. Which of the following combination of liquids form ideal mixture?
(A) acetone and chloroform
(B) benzene and toluene
(C) carbon tetrachloride and methyl alcohol
(D) water and ethyl alcohol
80. The molality of a solution containing 18 g of glucose (molar mass 180 g) in 500 g of water is
(A) 1 m (B) 0.5 m
(C) 0.2 m (D) 1.2 m
81. The ΔG for a reaction at 300 K is -16 kcal and ΔH is -10 kcal . The entropy of the reaction is
(A) 20 cal deg^{-1} (B) $86.6 \text{ cal deg}^{-1}$
(C) 166 cal deg^{-1} (D) 100 cal deg^{-1}
82. The pH of 10^{-3} M NaOH solution is
(A) 10 (B) 11
(C) 12 (D) 13

83. Water boils at 100°C . Molal elevation constant for water is $0.513\text{ K mol}^{-1}\text{ kg}$. What is the boiling point of a solution containing 6 g of glucose (mol. Mass 180) per 100 g of water?
- (A) 101.539°C (B) 100.017°C
(C) 100.153°C (D) 99.983°C
84. For the reaction $\text{A} + \text{B} \rightarrow \text{C} + \text{D}$, $\Delta H = -25\text{ kcal}$ and $\Delta S = 90\text{ cal deg}^{-1}$ at 27°C . The reaction
- (A) is reversible at 27°C
(B) is not feasible at 27°C
(C) represents equilibrium state at 27°C
(D) can occur only at temperature higher than 27°C
85. Which of the following is an example of extensive property?
- (A) temperature (B) pressure
(C) specific heat at constant volume (D) enthalpy
86. The latent heat of vaporization of water at 100°C is 540 cal g^{-1} . The change in entropy when one mole of water at 100°C is evaporated is
- (A) $260\text{ cal K}^{-1}\text{ mol}^{-1}$ (B) $26\text{ cal K}^{-1}\text{ mol}^{-1}$
(C) $160\text{ cal K}^{-1}\text{ mol}^{-1}$ (D) $360\text{ cal K}^{-1}\text{ mol}^{-1}$
87. In polar coordinates, the ranges of the variables are,
- (A) $r = -\infty$ to ∞ ; $\theta = 0$ to 2π (B) $r = -\infty$ to ∞ ; $\theta = 0$ to π
(C) $r = 0$ to ∞ ; $\theta = 0$ to 2π (D) $r = -\infty$ to ∞ ; $\theta = 0$ to 4π
88. For a two component solid-solid phase diagram with reactive system forming one product, the number Eutectic point(s) will be,
- (A) 0 (B) 1
(C) 2 (D) 3
89. Nernst- Einstein relates diffusion constant with
- (A) coefficient of viscosity (B) conductivity
(C) resistivity (D) drift mobility

90. The magnetic moment of a diamagnetic material is
- (A) positive value
 - (B) zero
 - (C) negative value
 - (D) complex quantity with nonzero real and imaginary parts
91. In extended Huckel method, which one of the following is true?
- (A) the sum of Mulliken bond orders for all bonds is the total number of electrons
 - (B) the sum of Mulliken charge densities of all atoms is the total no. of electrons
 - (C) the sum of both bond orders and charge densities is the total no. of electrons
 - (D) bond orders and charge densities have no correlation with the total no. of electrons
92. Hartree-Fock theory fails to include
- (A) internuclear repulsion
 - (B) overlap
 - (C) antisymmetry of wave functions
 - (D) correlation
93. Both Simple MO theory and simple VB theory gives identical results for
- (A) H_2
 - (B) H_2^+
 - (C) O_2
 - (D) F_2
94. The sum of one electron energies of all the occupied MOs will not give total energy in the case of
- (A) Huckel theory
 - (B) Extended Huckel theory
 - (C) Hartree-Fock theory
 - (D) None of the above
95. The energies of S-cis and S-trans butadiene is identical in the case of
- (A) Huckel theory
 - (B) Extended Huckel theory
 - (C) Hartree-Fock theory
 - (D) None of the above

96. The C-C bond in C_2 molecule has
- (A) one sigma and two pi bonds
 - (B) two pi bonds alone
 - (C) one sigma and three pi bonds
 - (D) one sigma, two pi and one delta bond
97. The geometry around sulphur in $>S=O$ is
- (A) planar
 - (B) pyramidal
 - (C) sometimes planar, sometimes pyramidal depending on the substituents
 - (D) none of the above
98. The sigma-pi separability of the Hamiltonian is impossible because of the nonseparability of
- (A) inter-nuclear repulsion terms
 - (B) nuclear-electron attraction terms
 - (C) electron-electron repulsions terms
 - (D) kinetic energy terms
99. The interaction between two fragment molecular orbitals depends on
- (A) symmetry
 - (B) overlap
 - (C) energy difference
 - (D) all of the above
100. The reference molecule for free valence in Huckel theory is
- (A) trimethylene methane
 - (B) benzene
 - (C) ethylene
 - (D) tetramethyl silane