

- The wave function Ψ associated with the motion of electron in a hydrogen atom can be expressed conveniently as a function of :
(A) Cartesian co-ordinates x, y, z (B) Spherical Polar co-ordinates r, θ, ϕ
(C) Cylindrical co-ordinates r, ϕ, z (D) None of these
- The major weakness of the Molecular Mechanics method is :
(A) It ignores electrons.
(B) The calculations are relatively slow.
(C) Gives poor results for IR spectra.
(D) Cannot be applied to molecules with more than 100 atoms.
- The ROHF method is used for which of the following molecules ?
(A) H_2O (B) CH_4 (C) O_2 (triplet) (D) BF_3
- Which of the following is a semi empirical quantum chemical molecular orbital method ?
(A) PX_4 (B) RHF/STO - 3G* (C) AMBER (D) AMI
- The number of atomic orbital(s) that hydrogen atom has is :
(A) Infinite (B) Zero (C) One (D) Two
- Which of the following statements is false about Valence Bond Theory ?
(A) It is a quantum mechanical approach
(B) The total wave function or trial wave function is the product of the individual bond eigen functions
(C) It makes no attempt to predict the shape of the molecules
(D) The individuality of the atoms are maintained
- In the Lyman series of the atomic hydrogen spectrum, the allowed transition is :
(A) $2P \rightarrow 2S$ (B) $2S \rightarrow 2D$ (C) $2F \rightarrow 2P$ (D) None of the above
- In the Hückel theory, the secular determinant has :
(A) Resonance integrals as the diagonal elements
(B) Coulomb integrals as the diagonal elements
(C) β as the diagonal elements
(D) Exchange integrals as the diagonal elements

9. In the rotational - vibrational spectrum of a molecule, the series observed towards the high frequency side is :
 (A) R branch (B) Q branch (C) P branch (D) None of the above

10. The character table for NH_3 molecule is given below :

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y) (R_x, R_y)$	$(x^2 - y^2, xy) (xz, yz)$

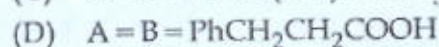
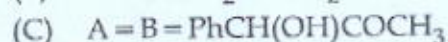
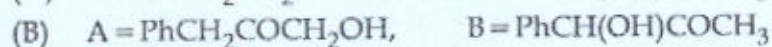
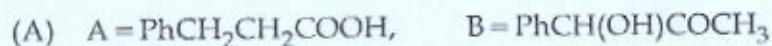
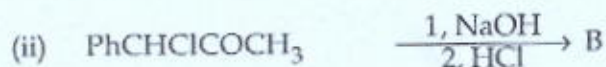
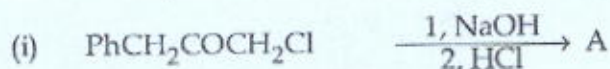
Which of the following statements is correct ?

- (A) The A_1 mode is infrared inactive
 (B) The A_1 mode is Raman inactive
 (C) The A_1 mode is infrared active but Raman inactive
 (D) The A_1 mode is both infrared and Raman active
11. The value of K_p and K_c are related by the equation :
 (A) $K_p = K_c (RT)^{\Delta n}$ (B) $K_p = K_c$ (C) $K_c = K_p (RT)^{\Delta n}$ (D) $K_p = K_c (RT)^{1/\Delta n}$
12. A line of constant composition in a phase diagram is _____.
 (A) A tie line (B) An isopleth
 (C) A eutectic halt (D) None of the above
13. The spontaneity of a process is favored when :
 (A) ΔH is (+), ΔS is 0 (B) ΔH is 0, ΔS is (+)
 (C) ΔH is (-), ΔS is (+) (D) ΔH is (-), ΔS is 0
14. The Helmholtz, - Smoluchowski equation is :
 (A) $\zeta = 4\pi\eta u / \epsilon_r$ (B) $\zeta = \frac{2}{3} \pi\eta u / \epsilon_r$ (C) $\zeta = 4\pi\eta \epsilon_r / u$ (D) $\zeta = \frac{2}{3} \pi \epsilon_r u / \eta$
15. The Ilkovic equation is used for the calculation of :
 (A) Voltage (B) Diffusion current
 (C) Electrode potential (D) None of the above

16. The number associated with the flow of fluid through a pipe of radius r is :
 (A) Gold number (B) Mole number
 (C) Reynold number (D) None of the above
17. The *Parke's process* is carried out for the purpose of :
 (A) Desilverization of lead (B) Determination of gold number
 (C) Purification of gold (D) None of the above
18. The *Mark - Houwink* equation shows the relationship between :
 (A) Viscosity and mass of the polymer
 (B) Viscosity and density of the polymer
 (C) The intrinsic viscosity and mass of the polymer
 (D) None of the above
19. At N.T.P., the viscosity of hydrogen is 8.4×10^{-5} poise and the average velocity of the molecules is 17×10^5 cm per sec. Calculate the mean free path if $\rho = 9 \times 10^{-5}$.
 (A) 1.647×10^5 cm (B) 1.8907×10^5 cm
 (C) 6.746×10^4 cm (D) 3.647×10^{10} cm
20. One mole of an ideal gas is heated from 100 K to 300 K. Calculate ΔS if (a) the volume is kept constant (b) the pressure is kept constant. Assume that $C_v = 1.5 R$.
 (A) $22.83 \text{ J K}^{-1} \text{ mol}^{-1}$; $13.70 \text{ J K}^{-1} \text{ mol}^{-1}$
 (B) $1.370 \text{ J K}^{-1} \text{ mol}^{-1}$; $2.283 \text{ J K}^{-1} \text{ mol}^{-1}$
 (C) $13.70 \text{ J K}^{-1} \text{ mol}^{-1}$; $22.83 \text{ J K}^{-1} \text{ mol}^{-1}$
 (D) $2.283 \text{ J K}^{-1} \text{ mol}^{-1}$; $1.370 \text{ J K}^{-1} \text{ mol}^{-1}$
21. Classify the following substituents as ortho - para or meta directing groups, if present on benzene ring in aromatic electrophilic substitution reaction.
 (i) CF_3 (ii) $\text{N}=\text{O}$ (iii) Br (iv) SO_3H
 (A) (i) ortho - para (ii) meta (iii) meta (iv) ortho - para
 (B) (i) meta (ii) meta (iii) ortho - para (iv) meta
 (C) (i) meta (ii) ortho - para (iii) meta (iv) ortho - para
 (D) (i) ortho - para (ii) ortho - para (iii) ortho - para (iv) meta
22. What is the value of n in Huckel's rule of aromaticity when a compound has 9 pairs of π electrons ? Predict whether such a compound is aromatic, anti-aromatic or non-aromatic.
 (A) $n=5$, non-aromatic (B) $n=4$, anti-aromatic
 (C) $n=4$, aromatic (D) $n=5$, aromatic

23. The following ester undergo hydrolysis by $B_{AC}2$ mechanism.
 $CH_3-CH_2-CO-O^{18}-CH_3$
 Which of the following products contain the O^{18} label ?
- (A) CH_3-CH_2-COOH (B) CH_3-CH_2-OH
 (C) CH_3-OH (D) CH_3-COOH
24. The simplest alkane which is optically active is :
- (A) 2 - methyl butane (B) 3 - methyl pentane
 (C) 2 - methyl hexane (D) 3 - methyl hexane
25. What will be the major product when 2 - methyl - 2 - butene reacts with each of the following :
- (i) $Hg(OAc)_2, H_2O$ followed by $NaBH_4$ and $NaOH$
 (ii) BH_3 , THF followed by H_2O_2 and $NaOH$
- (A) (i) 2 - methyl - 1 - butanol (ii) 3 - methyl - 2 - butanol
 (B) (i) 3 - methyl - 2 - butanol (ii) 2 - methyl - 1 - butanol
 (C) (i) 3 - methyl - 2 - butanol (ii) 2 - methyl - 2 - butanol
 (D) (i) 2 - methyl - 2 - butanol (ii) 3 - methyl - 2 - butanol
26. The correct order of stability of the following carbocations is :
- (A) methyl < primary alkyl < tertiary alkyl < benzyl
 (B) methyl < benzyl < primary alkyl < tertiary alkyl
 (C) tertiary alkyl < benzyl < primary alkyl < methyl
 (D) methyl < primary alkyl < benzyl < tertiary alkyl
27. The pK_a value of p - chloro benzoic acid is 3.98 and that of benzoic acid is 4.19. The calculated value of the substituent constant (σ_p) for the parachloro group is :
- (A) +0.21 (B) -0.21 (C) +0.0224 (D) -0.0224
28. Which of the following alkyl halide will undergo S_N2 ethanolysis fastest ?
- (A) Bromomethane (B) Bromoethane
 (C) Bromopropane (D) 2 - methyl - 1 - Bromo propane

29. Predict the product of the following rearrangement reactions.



30. The favoured conformation for 1, 2 - dichloroethane, 1, 2 - ethanediol and propanaldehyde are respectively :

(A) Gauche, anti, eclipsed

(B) Eclipsed, gauche, anti

(C) Anti, gauche, eclipsed

(D) Anti, eclipsed, gauche

31. Which of the following molecules will not show infrared spectrum ?

(A) H_2

(B) HCl

(C) H_2O

(D) CH_4

32. How many ESR lines are obtained from the compound CD_3 ?

(A) 3

(B) 4

(C) 6

(D) 7

33. ^{19}F NMR for HPF_2 molecule ($I_F = 1/2$) gives :

(A) 2 peaks

(B) 3 peaks

(C) 4 peaks

(D) 6 peaks

34. The number of degenerate levels for rotational level with rotational quantum number $J=4$ is :

(A) 8

(B) 9

(C) 33

(D) 10

35. Which of the following is not a common detector for gas chromatography ?

(A) Thermal conductivity detector

(B) Flame ionization detector

(C) Refractive index detector

(D) Mass spectrometer

36. The polymeric species $(\text{SN})_n$ is :

(A) Three dimensional conductor

(B) Insulator

(C) Two dimensional conductor

(D) One dimensional conductor

37. The principal reserve carbohydrate in animals is :

(A) Glucose

(B) Glycogen

(C) Sucrose

(D) Lactose

38. Myrcene belongs to :
 (A) Acyclic monoterpene (B) Cyclic diterpene
 (C) Acyclic diterpene (D) Bicyclic sesquiterpene
39. Diel's hydrocarbon is :
 (A) 1, 2 - cyclopentenophenanthrene
 (B) 2' - methyl - 1, 2 - cyclopentenophenanthrene
 (C) 3' - methyl - 1, 2 - cyclopentenophenanthrene
 (D) 3, 4 - cyclopentenophenanthrene
40. The transparent plastic is :
 (A) Polyurethane (B) Polycarbonates (C) Epoxy resin (D) Teflon
41. The compound that will behave as an acid in H_2SO_4 is :
 (A) H_2O (B) CH_3COOH (C) HNO_3 (D) $HClO_4$
42. The electronegativity difference is highest for the pair :
 (A) Li, Cl (B) Na, Cl (C) K, F (D) Li, F
43. Among the following orbitals of diatomic molecule, the bonding orbital is :
 (A) $1\sigma_u$ (B) $2\sigma_u$ (C) $1\pi_u$ (D) $1\pi_g$
44. Molecule with highest dipole moment is :
 (A) CH_3Cl (B) CH_2Cl_2 (C) $CHCl_3$ (D) CCl_4
45. Jahn Teller effect affects the geometry of :
 (A) $[Ni(NH_3)_6]^{2+}$ (B) $[Cu(NH_3)_4]^{2+}$ (C) $[MnCl_4]^{2-}$ (D) None of these
46. Optical isomerism is shown by :
 (A) $[Ni(CN)_4]^{2-}$ (B) $[Pt(NH_3)_4]^{2+}$ (C) $[Ni(CO)]_4$ (D) $[Co(en)_3]^{3+}$
47. The hybridisation of Xe in XeF_6 is :
 (A) dsp^3 (B) sp^3d (C) sp^3d^3 (D) sp^3d^2
48. The closeness of a result to its true or accepted value is :
 (A) Precision (B) Accuracy (C) Median (D) None of these

49. The metal which forms heteropoly acid is :
 (A) Ti (B) Zn (C) W (D) Cu
50. Which of the following complex ions shows the maximum intensity of absorption in UV - Visible region ?
 (A) $[\text{Cr}(\text{H}_2\text{O})_6]^{2+}$ (B) $[\text{V}(\text{H}_2\text{O})_6]^{2+}$ (C) $[\text{Co}(\text{H}_2\text{O})_6]^{2+}$ (D) $[\text{Mn}(\text{H}_2\text{O})_6]^{2+}$
51. Wittig reagent is :
 (A) $\text{Ph}_3\text{P}=\text{CH}_2$ (B) AlCl_3
 (C) $\text{CH}_3-\text{CH}=\text{CH}_2$ (D) $\text{HCO}(\text{CO})_3$
52. What is Ferrocene ?
 (A) Fe (B) Tris (cyclopentadienyl) iron
 (C) Bis (cyclopentadienyl) iron (D) FeSO_4
53. EAN value of $\text{Ni}(\text{CO})_4$ is _____.
 (A) 36 (B) 54 (C) 37 (D) 34
54. What is the function of cytochromes ?
 (A) Oxygen carriers (B) CO_2 carriers
 (C) Proton carriers (D) Electron carriers
55. Metal ion present in Chlorophyll is _____.
 (A) Fe (B) Mg (C) Ca (D) K
56. Give the equation for Geiger Nuttall rule :
 (A) $\log \lambda = A \log R + B$ (B) $M = Z(\text{MH}) + A - Z$
 (C) $N = N_0 e^{-\lambda d}$ (D) $\log R = \lambda(A + B)$
57. The bonding in Borane is _____.
 (A) two centre three electron (B) covalent
 (C) two centre two electron (D) three centre two electron
58. Identify the reaction in which Organoboranes are involved ?
 (A) Mannich reaction (B) Reimer - Tiemann reaction
 (C) Suzuki reaction (D) Henry reaction
59. Which is the main component of Portland Cement Clinker ?
 (A) Sodium silicate (B) Calcium silicate
 (C) Zinc silicate (D) Zirconium silicate

60. Give the general formula of Silanes :
 (A) Si_n (B) $\text{Si}_n\text{H}_{2n+2}$ (C) $\text{Si}_n\text{H}_{2n-2}$ (D) $\text{Si}_{2n+2}\text{H}_n$
61. Nanostructures have size in between :
 (A) 1 and 100 Å (B) 1 and 100 nm
 (C) 100 and 1000 nm (D) None of the above
62. The probe of Scanning Tunneling Microscope is as sharp as :
 (A) an atom at the tip (B) many atoms at the tip
 (C) a needle (D) none of the above
63. Quantum Dots are :
 (A) 1 dimensional (B) 2 dimensional (C) 0 dimensional (D) 3 dimensional
64. 12 - crown - 4 selectively bind with :
 (A) Li^+ (B) Na^+ (C) K^+ (D) None of these
65. Calixarenes are compounds that belong to the class of :
 (A) Crown ethers (B) Cryptands (C) Cyclophanes (D) Cyclodextrins
66. The anti-biotic which behaves like 'crown ethers' in promoting the K^+ transport across cell membrane is :
 (A) Nonactin (B) Pencillin (C) Tetracycline (D) None of these
67. The interior of cyclodextrins are :
 (A) Hydrophilic (B) Hydrophobic (C) Ionic (D) None of these
68. Crown ethers are best used as :
 (A) Homogeneous catalyst (B) Heterogeneous catalyst
 (C) Phase transfer catalyst (D) None of these
69. The first ionic liquid which is used as a green solvent is :
 (A) Ethyl Ammonium Nitrate (B) Methyl Ammonium Nitrate
 (C) Isopropyl Ammonium Nitrate (D) None of the above
70. The best green solvent is :
 (A) Super Critical NO_2 (B) Super Critical CO_2
 (C) Super Critical NH_3 (D) None of these

71. A good scientific research is characterized by :
- (A) It requires clear articulation of a goal
 - (B) It follows specific plan and procedure
 - (C) It accepts certain critical assumptions
 - (D) All the above
72. To understand human behavior and reasons over a long period of time one has to do :
- (A) Historical study
 - (B) Quasi experimental study
 - (C) Longitudinal study
 - (D) Cross sectional study
73. Teaching and learning arrangements, usually in small groups, that are structured to produce active participation in learning is :
- (A) Symposium
 - (B) Seminar
 - (C) Conference
 - (D) Workshop
74. Directly useful application of scientific principles to production is called :
- (A) Knowledge
 - (B) Science
 - (C) Technology
 - (D) Research
75. Which of the following qualities a researcher must have ?
- (A) Curious about the world
 - (B) Logical and systematic
 - (C) Intellectually honest
 - (D) All the above
76. The most effective teaching method that ensures maximum participation of students is :
- (A) Lecture method
 - (B) Text book method
 - (C) Discussion method
 - (D) Demonstration method
77. Which of the following is the most important indicator of quality of education in a school ?
- (A) Infrastructural facilities
 - (B) Qualification of teachers
 - (C) Discipline maintained in the school
 - (D) Students' achievements
78. Which of the following is not a quality of effective teacher ?
- (A) Less interaction in the class
 - (B) Adopt interactive method of teaching
 - (C) Reduce the anxiety level of students
 - (D) Motivate the students to take initiative