

一、 選擇題 (單選題，答案請填於答案卡，每題 2 分，無倒扣，共 100 分)

1. Please consider which type of atomic orbital is the following wave function belonging to?

$$\frac{1}{4} \sqrt{\frac{5}{\pi}} (3\cos^2\theta - 1)$$

(A) d_{z^2} (B) d_{xz} (C) d_{yz} (D) $d_{x^2-y^2}$ (E) d_{xy}

2. Which of the following descriptions for atomic structure is incorrect?

(A) The 2s orbital has a nodal surface. (B) The angular functions of atomic orbitals determine how the probability changes from point to point at a given distance from the center of the atom. (C) 3d orbitals have no radial nodes. (D) Coulombic energy depends on the number of possible exchanges between two electrons with the same energy and the same spin. (E) There are 3 angular nodes in f orbitals.

3. Please use Slater's rules to determine the effective nuclear charge of a 4s electron of Cu. The effective nuclear charge is

(A) 3.55 (B) 3.70 (C) 4.05 (D) 4.20 (E) none of above.

4. About the shape and geometry of molecules, which of the following descriptions is incorrect?

(A) The Cl-Sn-Cl bond angle in SnCl_2 is smaller than 120° .
 (B) XeF_4 is a square planar molecule.
 (C) In carbonyl fluoride COF_2 , the F-C-F angle is larger than the O-C-F angle.
 (D) ClF_3 has a T-shaped structure.
 (E) In XeOF_4 , no F atom is trans to the O atom.

5. Which of the following geometries is the correct one for SF_4 ?

(A) Tetrahedral (B) Seesaw (C) Square planar (D) Square antiprismatic (E) Square pyramidal

6. Which of the following molecules or ions has the same molecular geometry with H_2O ?

(A) N_3^- (B) CO_2 (C) SO_2 (D) XeF_2 (E) NO_2^+

7. What point group does osmocene $\text{Os}(\text{C}_5\text{H}_5)_2$ (eclipse) belong to?

(A) C_{2v} (B) D_{3h} (C) C_{5v} (D) D_{5h} (E) S_5

8. Which of the following molecule belongs to D_{2d} point group?

(A) Water H_2O (B) Carbon dioxide CO_2 (C) Ammonia NH_3 (D) Diborane B_2H_6
 (E) Allene $\text{H}_2\text{C}=\text{C}=\text{CH}_2$

9. Which of the following answers is the correct irreducible representation sum of the reducible representation Γ ?

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1
Γ	4	2	-2	0

(A) $A_1 + A_2 + B_1 + B_2$ (B) $2A_1 + B_1 + B_2$ (C) $3A_2 + B_1$ (D) $A_1 + 2A_2 + B_2$ (E) $A_2 + 2B_1 + B_2$

10. Which of the following descriptions is correct for $Mn(CO)_5Cl$?

C_{4h}	E	$2 C_4$	C_2	$2 \sigma_v$	$2 \sigma_d$	
A_1	1	1	1	1	1	z
A_2	1	1	1	-1	-1	Rz
B_1	1	-1	1	1	-1	
B_2	1	-1	1	-1	1	
E	2	0	-2	0	0	(x,y) (Rx,Ry)

- (A) $Mn(CO)_5Cl$ should have five IR-active stretching modes.
 (B) $Mn(CO)_5Cl$ should have three IR-active stretching modes from A_1 .
 (C) $Mn(CO)_5Cl$ should have two IR-active stretching modes from E.
 (D) $Mn(CO)_5Cl$ should have one IR-active stretching mode from B_1 .
 (E) $Mn(CO)_5Cl$ should have two IR-inactive stretching modes.

11. How many wave node planes can be found in δ^* orbitals?

(A) 3 (B) 4 (C) 5 (D) 6 (E) 7

12. Which of the following is the correct order for the internuclear distances of diatomic molecules/ions?

- (A) $N_2^{2-} > N_2^- > N_2 > N_2^+$ (B) $O_2^{2-} > O_2^- > O_2 > O_2^+$ (C) $N_2^+ > N_2 > N_2^- > N_2^{2-}$
 (D) $O_2^+ > O_2 > O_2^- > O_2^{2-}$ (E) None of above

13. Which of the following descriptions is correct for $KrBr^+$?

- (A) The electrons with highest energy are in π orbitals. (B) The HOMO is polarized toward Br.
 (C) The bond order equals 2. (D) Br is more electronegative than Kr. (E) None of above.

14. If z axis goes through A-B bond of molecule AB, please consider which of the following combination of atomic orbitals from atom A and atom B cannot form chemical bonding?

(A) p_x and d_{xz} (B) s and d_{z^2} (C) p_z and $d_{x^2-y^2}$ (D) d_{z^2} and p_z (E) $d_{x^2-y^2}$ and $d_{x^2-y^2}$

15. Which of the following molecules/ions can be a Lewis acid?

(A) Hexane (B) Borane (C) Dinitrogen (D) SbF_6^- (E) Diethyl ether

16. Which of the following molecules is the strongest base in aqueous solution?

(A) NH_3 (B) NH_2Me (C) $NHMe_2$ (D) NMe_3 (E) NH_2Ph

17. Which of the following answers shows the correct order of solubility in water for lead compounds?

(A) $PbS > PbI_2 > PbBr_2 > PbCl_2$ (B) $PbI_2 > PbBr_2 > PbCl_2 > PbS$

(C) $PbS > PbCl_2 > PbBr_2 > PbI_2$ (D) $PbCl_2 > PbBr_2 > PbI_2 > PbS$

(E) $PbBr_2 > PbCl_2 > PbS > PbI_2$

18. Which of the following unit cells belongs to D_{4h} point group?

(A) Body-centered tetragonal (B) Face-centered cubic (C) Diamond (D) $CsCl$

(E) Nickel arsenide

19. Which of the following electron configurations is incorrect?

(A) V: $[Ar]4s^23d^3$ (B) Cr: $[Ar]4s^23d^4$ (C) Mn: $[Ar]4s^23d^5$ (D) Ni: $[Ar]4s^23d^8$

(E) Zn: $[Ar]4s^23d^{10}$

20. In C_{2v} point group, x and y coordinates belong to which of the following representations?

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

(A) A_1 and A_2 (B) A_2 and B_1 (C) A_1 and B_1 (D) A_2 and B_2 (E) B_1 and B_2

21. Which of the following answers includes only hard acids?

(A) Al^{3+} , Ag^+ (B) H^+ , K^+ (C) Cu^+ , I_2 (D) CO , Zn^{2+} (E) $Tl(CH_3)_3$, Cr^{3+}

22. Which of the following descriptions for sulfur is incorrect?
- (A) The most stable form at room temperature is α -S₈.
(B) The viscosity of sulfur decreases as the temperature increases from 120 °C to 300 °C.
(C) Sulfur can form linear long chain structure.
(D) SO₃ can be absorbed easily by sulfuric acid.
(E) Peroxodisulfate is a useful oxidizing agent.
23. Which of the following descriptions for xenon is incorrect?
- (A) Xe can be reduced by PtF₆ to form XeF⁺. (B) Xenon can be a ligand for Au²⁺.
(C) The number of lone pairs on Xe in XeF₄ is 2. (D) XeF₄ has a square planar geometry.
(E) Xe-N and Xe-C bonds can be found in some compounds.
24. Which of the following descriptions for carbon is incorrect?
- (A) Potassium atoms can be intercalated between graphite layers to form a strong reducing agent.
(B) The point group of Buckminsterfullerene C₆₀ is I_h.
(C) The crystal structure of calcium carbide, CaC₂, resembles that of NaCl.
(D) 5-Coordinate carbon can be found in some alkyl metal compounds.
(E) Graphyne is constructed by carbon atoms with only single and double bonds.
25. Please select the correct oxidation states for nitrogen in the following compounds: NH₃OH⁺, NO, N₂O₄.
- (A) -2, +1, +4 (B) -1, +1, +3 (C) -2, +2, +3 (D) -1, +2, +4 (E) None of above.
26. The number of possible pairs of enantiomers for the formula M(ABA)cde? ABA is a tridentate ligand and c, d, e are a monodentate ligand.
- (A) 1 (B) 2 (C) 3 (D) 4 (E) 5
27. The coordination number of Au in complex [(Et₃P)AuTi(CO)₆]⁻ is 2. What is the geometry in Ti atom?
- (A) Octahedral (B) Capped trigonal prismatic (C) Capped octahedral
(D) Pentagonal bipyramidal (E) Square pyramidal
28. Which one of the following complexes is pentagonal planar?
- (A) Ni(CN)₅³⁻ (B) Cu(NH₃)₅²⁻ (C) VO(acac)₂ (D) CuCl₅³⁻ (E) XeF₅

29. The ReH_9^{2-} has a geometry of
(A) Tricapped trigonal prism (B) Capped square antiprism (C) Capped octahedron
(D) Trigonal dodehedron (E) None of above
30. Determine the exchanging energies for high spin d^6 ions in an octahedral complex.
(A) $1\text{P}\epsilon$ (B) $2\text{P}\epsilon$ (C) $3\text{P}\epsilon$ (D) $4\text{P}\epsilon$ (E) $5\text{P}\epsilon$
31. On the basis of VSEPR, which of the following point group is NOT correct?
(A) XeOF_2 is C_{2v} (B) XeOF_4 is C_{4v} (C) XeO_2F_2 is D_{2h} (D) XeO_3F_2 is D_{3h} (E) All correct
32. HXeO_4^- ion obtained from XeO_3 in basic solution; this ion subsequently undergoes disproportionation reaction in basic OH^- , $2\text{HXeO}_4^- + 2\text{OH}^- \rightarrow$ products. Which one of the following is NOT one of the products?
(A) Xe (B) HXeO_6^{3-} (C) XeO_6^{4-} (D) O_2 (E) H_2O
33. Which one of the following structure is NOT geometry as pentagonal bipyramid(PBP)?
(A) IF_7 (B) $\text{UO}_2\text{F}_5^{3-}$ (C) NbOF_6^{3-} (D) NiF_7^{3-} (E) None of above
34. Which one of the following structures is considered as "See-saw"?
(A) IF_2O_2^- (B) IOF_3 (C) ClF_4^+ (D) XeO_2F_2 (E) All of above
35. Glycine has the structure $\text{NH}_2\text{CH}_2\text{COOH}$. It can lose a proton from the carboxyl group and form chelate rings bonded through both N and one the O atoms. How many possible isomers of tris(glycinato)cobalt(III)?
(A) 3 (B) 4 (C) 5 (D) 6 (E) 8
36. The d^2 ions CrO_4^{4-} , MnO_4^{3-} , FeO_4^{2-} and RuO_4^{2-} have been reported. Which of following statements is false?
(A) Complex RuO_4^{2-} has the largest value of Δ_t . (B) Complex FeO_4^{2-} has the shortest metal-oxygen distance. (C) The nuclear charge of iron is greatest in this isoelectronic series.
(D) These are LMCT absorption. (E) All of above.
37. What is the ground term for low-spin d^4 ions? Which one of the following is correct?
(A) Its configuration is $t_{2g}^4 e_g^0$. (B) Spin multiplicity is 3. (C) Highest possible value of M_L is 5.
(D) The ground term is 3H . (E) All of above.
38. Which one of the following complexes is high spin?
(A) $\text{Cr}(\text{CN})_6^{4-}$ (B) $\text{Fe}(\text{H}_2\text{O})_6^{2+}$ (C) $\text{Fe}(\text{CN})_6^{4-}$ (D) $\text{Co}(\text{NH}_3)_5(\text{H}_2\text{O})^{3+}$ (E) None of above

39. A wide variety of ligands can kinetically stabilize ions that would normally be potent oxidizing agents. Which of the following statements is NOT correct for an example of Co(III)-Co(II) couple?
- (A) Co(III) is kinetically stable when coordinated with any ligand other than water or fluoride.
(B) The hydrated $\text{Co}(\text{H}_2\text{O})_6^{3+}$ is a very strong oxidizing agent, reacting readily with water to form H_2 and Co(II).
(C) The oxidation of a Co(II) complex to a Co(III) complex generally results in a change from the high-spin Co(II) to the low-spin Co(III) accompanied by a significant increase in LFSE with almost any ligand.
(D) The case in (C) often contributes to the stability of many Co(III) complexes, rendering many of them weaker oxidizing agents than expected.
(E) None of above.
40. Which one of the following complexes is *labile*?
- (A) $\text{Cr}(\text{CN})_6^{4-}$ (B) $\text{Fe}(\text{CN})_6^{3+}$ (C) $\text{Cr}(\text{H}_2\text{O})_6^{2+}$ (D) MnI_6^{2-} (E) $\text{Ru}(\text{NH}_3)_6^{2+}$
41. Predict the numbers of C-O and C-N stretches in *cis*- $[\text{Fe}(\text{CO})_2(\text{CN})_4]^{2-}$.
- (A) 2, 3 (B) 2, 4 (C) 1, 3 (D) 2, 1 (E) 2, 2
42. The NO (nitrosyl) ligand shares many similarities with CO. Which of the following statements is NOT correct?
- (A) Like CO, it's a σ donor and π acceptor and can serve as terminal or bridging ligand.
(B) NO has two common coordination modes; linear and bent.
(C) Linear NO is counted as a 2-electron donor, same as CO.
(D) $\text{Fe}(\text{CN})_5(\text{NO})^{2-}$ has been used as a vasodilator for the treatment of high blood pressure.
(E) $\text{Cr}(\text{NO})_4$ is tetrahedral molecule.
43. All five complexes followed 18E rule. Which one has the largest ν_{CO} ?
- (A) $\text{Ti}(\text{CO})_6^{2-}$ (B) $\text{V}(\text{CO})_6^-$ (C) $\text{Cr}(\text{CO})_6$ (D) $\text{Mn}(\text{CO})_6^+$ (E) $\text{Fe}(\text{CO})_6^{2+}$
44. What is the bond order in complexes $\text{Cp}_2\text{Mo}_2(\text{CO})_4$?
- (A) 1 (B) 1.5 (C) 2 (D) 2.5 (E) 3
45. How many bridging μ -CO in $\text{Ir}_4(\text{CO})_{12}$?
- (A) 0 (B) 1 (C) 2 (D) 3 (E) 4

46. The reaction of $\text{Re}(\text{CO})_5\text{Br}$ with the ion $\text{BrCH}_2\text{CH}_2\text{O}^-$ gave compound **Y** and Br^- . Which one the following statement is NOT correct.

- (A) The most likely site of attack of this ion is Re metal.
- (B) **Y** obeys 18e rule.
- (C) No gas is evolved in the reaction.
- (D) Addition of solution of Ag^+ to a solution of **Y** gave a white ppt.
- (E) ^{13}C NMR indicates there are five distinct magnetic environments for carbon in **Y**.

47. Upon heating, the complex $(\text{CO})_3\text{Mn}(\text{PPh}_3)_2(^{13}\text{COMe})$ lost a gas, what is the gas?

- (A) ^{12}CO (B) ^{13}CO (C) ^{12}CO and ^{13}CO (D) Me^{13}COH (E) None of above

48. What is Wilkinson's catalyst?

- (A) $\text{HRh}(\text{CO})_2(\text{PPh}_3)_2$ (B) $[\text{I}_2\text{Rh}(\text{CO})_2]^-$ (C) *cis*- $\text{IrCl}(\text{CO})(\text{PPh}_3)_2$ (D) *trans*- $\text{IrCl}(\text{CO})(\text{PPh}_3)_2$
- (E) $\text{RhCl}(\text{PPh}_3)_3$

49. The β abstraction of $\text{CpFe}(\text{CO})_2(\text{CMe}_2\text{D})$ by $[\text{Ph}_3\text{C}]^+[\text{BF}_4]^-$ gave major product $\text{CpFe}(\text{CO})_2(\text{DMeC}=\text{CH}_2)^+$ and **Y**. What is **Y**?

- (A) $\text{Ph}_3\text{C-H}$ (B) $\text{Ph}_3\text{C-D}$ (C) $\text{CH}_2=\text{CDMe}$ (D) $\text{MeCD}=\text{CD}_2$ (E) None of above

50. The reaction of $\text{Cp}_2\text{Sc}(\text{CH}_3) + \text{C}_6\text{H}_6 \rightarrow \text{Cp}_2\text{Sc}(\text{C}_6\text{H}_5) + \text{CH}_4$ is best described as

- (A) Oxidative addition (B) Reduction elimination (C) Nucleophilic displacement
- (D) Sigma bond metathesis (E) None of above