系所組別： 化學系

考試科目： 無機化學

※ 考生請注意：本試題 ■可 □不可 使用計算機

I. 單選題，每題答對得四分，答錯扣一分。(60%)

1. Using the Slater's rules, calculate Z* for a 4s electron in Zn (Z=30).
(A) 5.85 (B) 4.85 (C) 4.70 (D) 4.35 (E) 3.90

2. What is the point group for the *fac*-$[FeCl_3(CN)_3]^{3-}$ ion?
(A) O_h (B) D_{3d} (C) C_{3v} (D) C_3 (E) C_s

3. What is the point group for the cubane, C_8H_8?
(A) D_{2h} (B) D_{2d} (C) D_{3d} (D) T_d (E) O_h

4. How many ^{13}C NMR signals do you expect to see for C_{60} and C_{70}, respectively?
(A) 1, 2 (B) 2, 2 (C) 1, 5 (D) 3, 3 (E) 3, 5

5. How many ion pairs are there in the unit cell of NaCl and ZnS (zinc blende) structure, respectively?
(A) 4, 4 (B) 4, 1 (C) 4, 2 (D) 1, 4 (E) 1, 2

6. Which of the following carbonates has the highest enthalpy of decomposition?
(A) Na_2CO_3 (B) K_2CO_3 (C) $BeCO_3$ (D) $CaCO_3$ (E) $SrCO_3$

7. The best Lewis structure for NCO^-, where the arrangement of atoms is N-C-O, the formal charges on N, C, and O, respectively, are
(A) -2, 0, +1 (B) -1, +1, -1 (C) -2, +1, 0 (D) -1, 0, 0 (E) 0, 0, -1

8. Which of hybridization for the central atom is incorrect?
(A) NO_2: sp^2 (B) SF_5: sp^3d^2 (C) ClF_3: sp^3d (D) SbH_3: sp^3 (E) SF_4: sp^3d

9. Which of following complexes has spinel structure?
(A) Mn_3O_4 (B) $MnFe_2O_4$ (C) Fe_3O_4 (D) $NiAl_2O_4$ (E) $MgFe_2O_4$

10. What is the effective moment μ_B in high temperature for a spin-crossover complex $[Fe(phen)_2(NCS)_2]$?
(A) 2.83 (B) 3.46 (C) 3.87 (D) 4.47 (E) 4.90

11. Which of the following complexes has the largest ligand field stabilization energy?
(A) $[CoCl_4]^{2-}$ (B) $[Co(NH_3)_6]^{3+}$ (C) $[Fe(H_2O)_6]^{3+}$ (D) $[Rh(NH_3)_6]^{3+}$ (E) $[Ti(H_2O)_6]^{3+}$

12. Determine the number of stereoisomers and number of pairs of enantiomers for an octahedral $M(a_2b_2c_2)$ complex, respectively? (a, b, and c are monodentate ligands.)
(A) 6, 1 (B) 4, 2 (C) 5, 1 (D) 7, 2 (E) 8, 2

13. Which of the following complexes has the strongest W-C bond which is *trans* to phosphine or phosphite ligand?
(A) $W(H_3P)(CO)_5$ (B) $W(F_3P)(CO)_5$ (C) $W(Br_3P)(CO)_5$ (D) $W(Ph_3P)(CO)_5$ (E) $W(PhO_3P)(CO)_5$

14. Which of the following ligands is the best *trans*-directing in the substitution reactions in the square planar complexes?
(A) H^- (B) CH_3^- (C) CN^- (D) Cl^- (E) SCN^-

15. Which of following species is isolobal with CH?
(A) $Fe(CO)_3$ (B) $Co(CO)_3$ (C) $Ni(CO)_3$ (D) $Fe(CO)_2(C_5H_5)$ (E) $Co(C_5H_5)$

(背面仍有題目,請繼續作答)

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II. 簡答題(40%)

1. Which of the following molecules is (are) optically active? (4%)

a: SClFO; b: SiF_2C_2; c: $[Co(en)_3]^{3+}$; d: $[Co(edta)]^-$; e: *cis*-$[CoCl_2(en)_2]^+$; f: *cis*-$[PtCl_2(NH_3)_2]$

2. a. Draw energy band pictures for metal, semiconductor and insulator. (3%)

b. $(Zr_{1-x}Ca_x)O_2$ ($0.1 \leqq x \leqq 0.2$, $T > 1000$ ℃) is found to exhibit significant electrical conductivity at indicated temperatures and compositions. Identify the species and mechanism that is responsible for electrical conduction. (3%)

3. a. Using the C_{3v} character table to predict infrared-active carbonyl stretching bands for $(\eta^6\text{-}C_6H_6)W(CO)_3$.(4%)

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	$(x,y)(R_x,R_y)$	$(x^2-y^2)(xz,yz)$

b. How will the IR and Raman spectra of F-H-F$^-$ and Cl-H-F$^-$ differ? (2%)

4. Construct the Born-Haber cycle for KBr crystal, and indicate all the name of enthalpy change (ΔH) you used. Use the date given in the following to calculate the lattice energy of KBr. (5%)

Formation enthalpy of KBr　ΔH_f = -393.8 KJ/mol

Sublimation energy of K　ΔH_{sub} = 89.2 KJ/mol

Dissociation energy of Br_2　ΔH_{dis} = 223.6 KJ/mol

Ionization energy of K　ΔH_{IE} = 418.4 KJ/mol

Electron affinity of Br　ΔH_{EA} = 324.6 KJ/mol

5. BeH_2 is linear. Draw the molecular orbitals to descript the bonding in BeH_2. (5%)

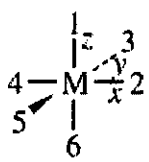
6. Both ^{19}F and ^{31}P have I = 1/2.

^{19}F NMR spectra of PCl_2F_3 at -22 °C and -143 °C are given.

a. What is the structure of PCl_2F_3 at -143 °C? (2%)

b. Explain the mechanism that causes the given spectrum. (4%)

7. Using the angular overlap method, determine the relative energies of d orbitals in terms of e_σ and e_π for an octahedral ML_6 complex. Assume that the ligands are capable of σ-donor and π-acceptor. (8%)



Octahedral positions

	Sigma Interactions (all in units of e_σ) Metal d Orbital					*Pi Interactions (all in units of e_π) Metal d Orbital*				
Ligand Position	z^2	x^2-y^2	xy	xz	yz	z^2	x^2-y^2	xy	xz	yz
1	1	0	0	0	0	0	0	0	1	1
2	1/4	3/4	0	0	0	0	0	1	1	0
3	1/4	3/4	0	0	0	0	0	1	0	1
4	1/4	3/4	0	0	0	0	0	1	1	0
5	1/4	3/4	0	0	0	0	0	1	0	1
6	1	0	0	0	0	0	0	0	1	1