編號： 57　系所：化學系　　科目：無機化學

本試題是否可以使用計算機： □可使用 ， ☑不可使用 （請命題老師勾選）

I 單選題 每小題 3 分

1. The rate constants for the exchange reaction, $CrX^{2+} + {}^*Cr^{2+} \rightarrow {}^*CrX^{2+} + Cr^{2+}$ where *Cr is radioactive ^{51}Cr, are given in the table for the reaction at 0°C and 1 M $HClO_4$. What is the probable mechanism for this reaction? A) outer-sphere mechanism B) inner-sphere mechanism

X^-	k ($M^{-1}s^{-1}$)
F^-	1.2×10^{-3}
Cl^-	11
Br^-	60
NCS^-	1.2×10^{-4}
N_3^-	>1.2

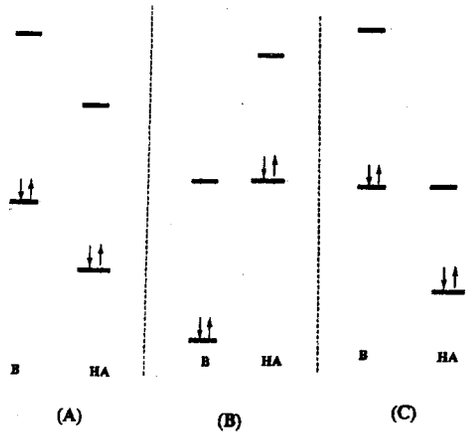
2. Which of the following metalloproteins does not play the role for electron transfer?

A) iron sulfur protein B) cytochrome a C) blue copper protein D) Coenzyme B_{12}

3. How many microstates for an s^1p^1 configuration?

A) 10 B) 12 C) 14 D) 16

4. B and HA form strong unsymmetrical hydrogen bonding. Which one is the possible frontier MO diagrams for B and HA?



5. What is the order of acidity in gas phase? (A) $SiH_4 < PH_3 < H_2S < HCl$ (B) $SiH_4 > PH_3 > H_2S >$ HCl (C) $PH_3 < H_2S < HCl < SiH_4$ (D) $H_2S < HCl < SiH_4 < PH_3$

6. Which of the following is not the Lattice point of a faced centered cubic structure?

A) (0,0,0) B) (1/2, 1/2, 0) C) (1/2, 1/2, 1/2) (D) (1/2, 0, 1/2) E) (0, 1/2, 1/2)

7. Which of the following material might be an n-type semiconductor?

A) arsenic doped silicon B) increasing the amount of S in Cu_2S C) gallium-doped silicon

（背面仍有題目,請繼續作答）

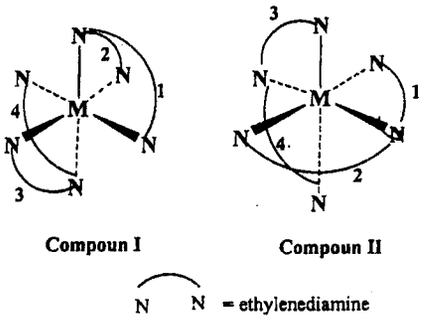
8. According to the figure on the right, which of the following statements is not correct?

(A) compound I is a facial form

(B) compound II is a meridional form

(C) compounds I and II are geometric isomers

(D) compound I and II are optical isomers



9. The combination of the chelate rings might cause chiral character. Please assign the absolute configuration for the combination of "ring 1" and "ring 3" in compound I (see the figure on the right). A) Λ B) Δ C) λ D) δ

10. Which metal shown below has the most affinity for binding to the amino acid, methionine?

(A) Hg^{2+}, (B) Cu^{2+}, (C) Co^{3+}, (D) Fe^{2+}

11. Which C-C distance of the following molecules is closer to the C-C distance of C_2^{2-} ? A) benzene, B) C_2H_4, C) C_2H_2 D) C_2H_6

12. Please order the bond dissociation energy for the following species C_2^+, C_2, C_2^-

A) $C_2^- > C_2 > C_2^+$　　B) $C_2^+ > C_2 > C_2^-$　　C) $C_2^- \approx C_2 \approx C_2^+$

II 簡答題　每小題 3 分

1. Determine the ground term of a high-spin d^7 configuration in O_h symmetry

The electronic spectrum of $[M(H_2O)_6]^{n+}$ and the simplified Tanabe-Sugano Diagrams in octahedral ligand field are shown in the last two pages. Please answer questions 2-5.

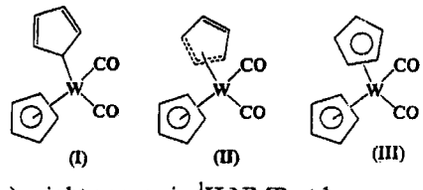
2. Please indicate the term of the ground state for $[Cr(H_2O)_6]^{2+}$

3. Please indicate the term of the ground state for $[Fe(CN)_6]^{4-}$

4. Please indicate the possible transition for $[Cr(H_2O)_6]^{3+}$

5. Please calculate Δo for $[Cr(H_2O)_6]^{2+}$ (B = 700 cm^{-1})

Please answer questions 6-8 regarding to compounds I, II, and III in the figure on the right

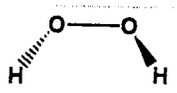


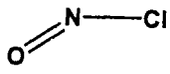
6. Determine the valence electrons for compounds I, II, and III.

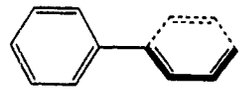
7. How many sets of peaks (do not consider hyperfine interaction) might appear in ^1H NMR at low temperature in compounds I, II, and III?

8. Please write down the ratio of peak intensity for compound I.

Please assign the point groups of the molecules in questions 9-11.

9. 

10 

11 

12. Which of molecules in "questions 9-11" is(are) chiral?

The point group of $[Co(ethylenediamine)_3]^{3+}$ is D_3, please complete the character table of this point group and answer questions 13-17.

	E	b	c
A_1	1	1	1
a	d	e	f
E	2	h	i

13. What is the label "a"?

14. What is (b, c)?

15. What is (h, i)?

16. What is the irreducible representation for *z* coordinate in this point group?

17. What is the irreducible representation for ***Rz*** (rotation of z axis) in this point group?

18. Please write down the reaction catalyzed by superoxide dismutase (SOD)

III　此題共 10 分 每一子題 2 分

Answer the following questions regarding to H_3^+ ion

a. Sketch the energy levels and the molecular orbitals for the H_3^+ ion, using **linear geometry**.

b. Include the symmetry labels for the orbitals.

c. The wave function of each MO (assume three atomic orbitals of three hydrogens are Ha, Hb, and Hc)

d. Indicate the HOMO and LUMO in your MO diagram.

e. Please describe the bonding of H_3^+ with the MO approach.

D_{2h}	*E*	$C_2(z)$	$C_2(y)$	$C_2(x)$	*i*	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	−1	−1	1	1	−1	−1	R_z	xy
B_{2g}	1	−1	1	−1	1	−1	1	−1	R_y	xz
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

(背面仍有題目,請繼續作答)

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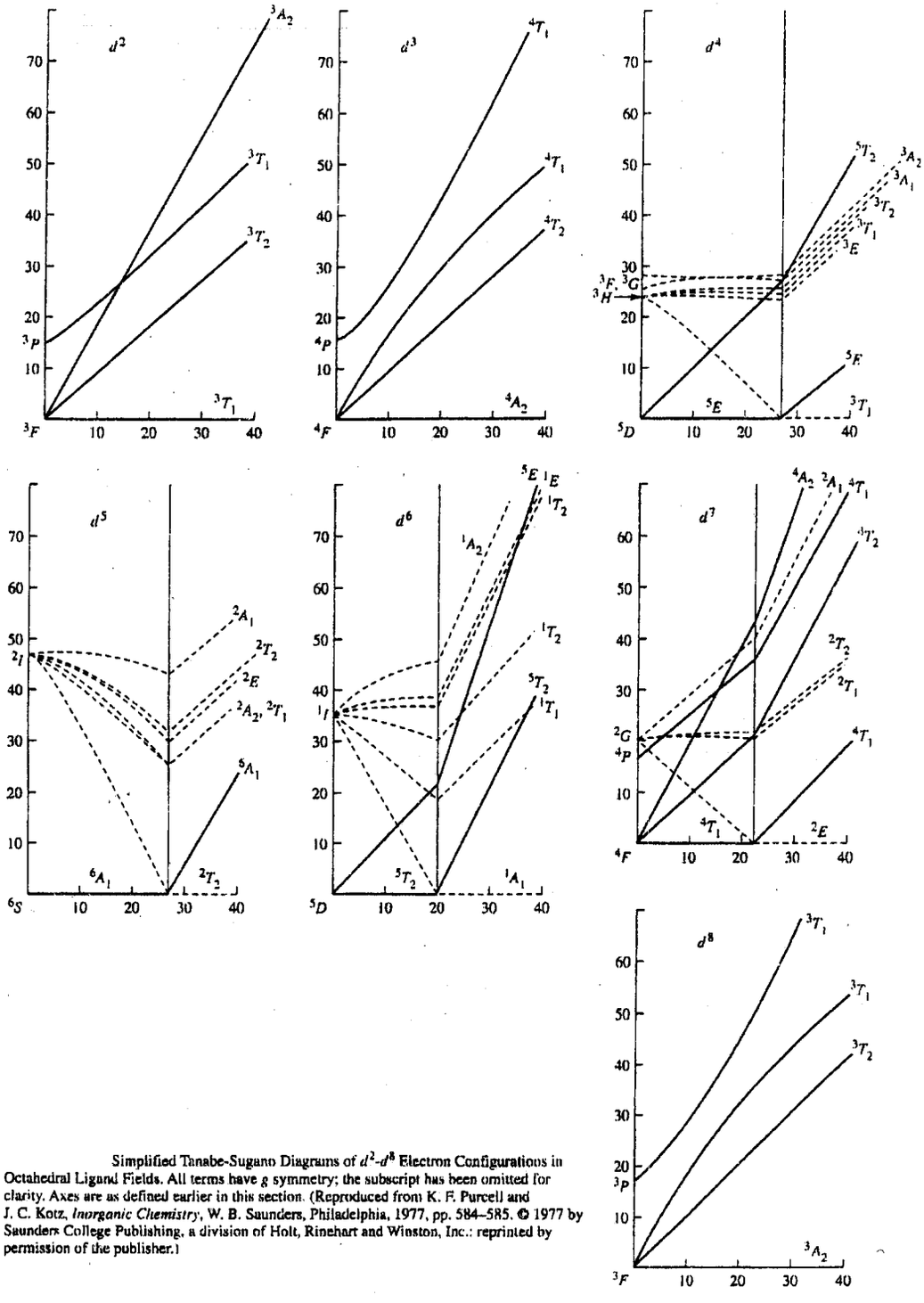

Simplified Tanabe-Sugano Diagrams of d^2-d^8 Electron Configurations in Octahedral Ligand Fields. All terms have g symmetry; the subscript has been omitted for clarity. Axes are as defined earlier in this section. (Reproduced from K. F. Purcell and J. C. Kotz, *Inorganic Chemistry*, W. B. Saunders, Philadelphia, 1977, pp. 584–585. © 1977 by Saunders College Publishing, a division of Holt, Rinehart and Winston, Inc.: reprinted by permission of the publisher.)

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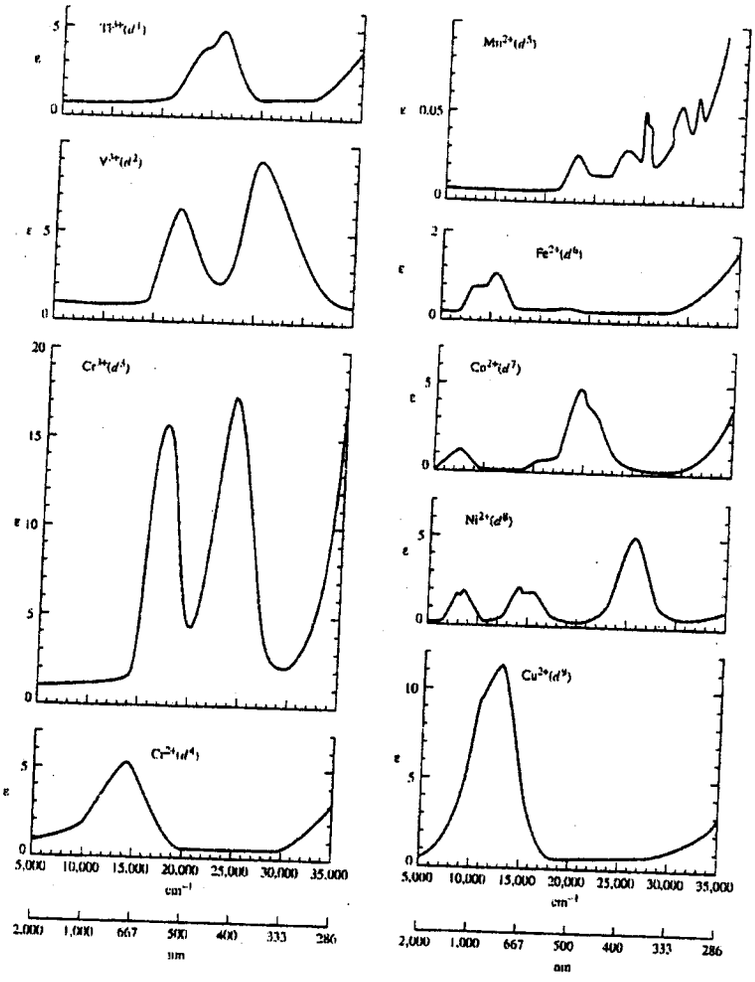

Electronic Spectra of First-Row Transition Metal Complexes of Formula $[M(H_2O)_6]^{n+}$. (Reproduced with permission from B. N. Figgis, *Introduction to Ligand Fields*, Wiley-Interscience, New York, 1966. pp. 221, 224.)