題號: 76

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Part I 與 Part II 分開作答 答案須清楚標示題號

Part I: (Total score 50%)

A: Multiple Choices 多選題(答錯倒扣)填答於答案紙上 (20%)

- 1. Which of the following term symbols belong to the electronic configuration of f^2 (a) 3 H (b) 3 G (c) 1 F (d) 1 D (e) 1 P
- 2. Which of the following molecules or ions have sp^3 hybridization and formal charge of +1 for the central atom:
 - (a) NO_3^- (b) BF_4^- (c) $S_2O_3^{2-}$ (d) ICl_2^+ (e) ClO_3^-
- 3. Among the following diatomic molecules, which of them have multiple bonds
 - (a) B_2 (b) C_2 (c) Li_2 (d) O_2^+ (e) F_2
- 4. Two fragments are isolobal if their highest energy orbitals have the same symmetry, similar energies and the same electron occupation. Which of the following fragments conform with isolobal analogy:
 - (a) CH (b) CH₂ (c) Co(CO)₃ (d) Co(CO)₄ (e) HFe(CO)₃

B:

- 5. Using the character table of D_{3h} shown below, derive irreducible representations for the three σ bonds of BF₃, and using projection operator method to find the group orbitals for each representation. 10%
- 6. Olefin metathesis is now a day an important process for the preparation of various organic compounds and polymers. Cyclohexene undergoes Ring Opening Metathesis Polymerization (ROMP) with a catalyst R₃Al/WCl₆ producing a polymer. Draw structure of the product and write a mechanism of polymerization. 10%
- 7. Explain briefly the following terms: 10%
- (a) Spectrochemical series (b) phosphorescence (c) oxidative addition (d) amphoterism (e) Hund's rule Part II: (Total score 50%)
- 8. Give proper explanations for the following observation. (10%)
- (a) O₂ is a paramagnetic compound.
- (b) HClO₂ is a weak acid, while HClO₄ is a strong acid
- (c) CCl₄ does not react with water, but SiCl₄ reacts with water to form SiO₂.
- (d) At room temperature, CO₂ is a gas but SiO₂ is a solid.
- (e) Diamond is one of the hardest materials, but graphite is often used as a lubricant.
- Indicate the <u>coordination numbers</u> of the cations and anions in the following solids, and calculate the <u>density</u> for each solid.
- (a) sodium iodide (NaCl structure; $r_{Na+} = 102$ pm, $r_{I^-} = 220$ pm; atomic weight of Na = 23.0, atomic weight of I = 126.9) (5%)
- (b) cesium bromide (CsCl structure; $r_{Cs^+} = 170$ pm, $r_{Br^-} = 196$ pm; atomic weight of Cs = 132.9, atomic weight of Br = 79.9) (5%)
- 10. Given the reduction potential $E_A{}^0 = 0.771 \text{ V for Fe}^{3+} + \text{e}^{-} \rightarrow \text{Fe}^{2+}$ (where A represents at [H⁺] = 1 M condition) and $Ksp = 4.87 \times 10^{-17}$ and 2.79×10^{-39} for Fe(OH)₂ and Fe(OH)₃, respectively.
- (a) Write the Nernst equations for the two half reactions: $Fe^{3+} \rightarrow Fe^{2+}$ and $Fe(OH)_3 \rightarrow Fe(OH)_2$.
- (b) What is reduction potential E_B^0 for the Fe(OH)₃ \rightarrow Fe(OH)₂ couple (where B represents at [OH] = 1 M condition)? (6%)
- 11. The Mn²⁺(aq) ion is pale pink, but the MnO₄⁻ ion is deep purple. Characterize the origins of the transitions and explain the relative intensities. (10%)

國立台灣大學九十四學年度碩士班招生考試試題

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12. Using the descending of symmetry if necessary, find the term symbols for the following electron configurations in octahedral crystal field. (10%)

(a) $t_{2g}^{i}e_{g}^{i}$

(b) e_g²

Correlation table

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	CONTONUE ON TOOLS	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	O _h	C _{2y}
$\begin{array}{cccc} E_{g} & A_{1} + A_{2} \\ T_{1g} & A_{2} + B_{1} + B_{2} \\ T_{2g} & A_{1} + B_{1} + B_{2} \\ A_{1u} & A_{2} \\ A_{2u} & A_{1} \\ E_{u} & A_{1} + A_{2} \\ T_{1u} & A_{1} + B_{1} + B_{2} \end{array}$	Alg	
$\begin{array}{cccc} E_{g} & A_{1} + A_{2} \\ T_{1g} & A_{2} + B_{1} + B_{2} \\ T_{2g} & A_{1} + B_{1} + B_{2} \\ A_{1u} & A_{2} \\ A_{2u} & A_{1} \\ E_{u} & A_{1} + A_{2} \\ T_{1u} & A_{1} + B_{1} + B_{2} \end{array}$	A_{2g}	A ₂
$\begin{array}{ccc} T_{2g} & A_1 + B_1 + B_2 \\ A_{1u} & A_2 \\ A_{2u} & A_1 \\ E_u & A_1 + A_2 \\ T_{1u} & A_1 + B_1 + B_2 \end{array}$	$\mathbf{E}_{\mathbf{g}}$	$A_1 + A_2$
$\begin{array}{ccc} T_{2g} & A_1 + B_1 + B_2 \\ A_{1u} & A_2 \\ A_{2u} & A_1 \\ E_u & A_1 + A_2 \\ T_{1u} & A_1 + B_1 + B_2 \end{array}$	$\mathrm{T_{lg}}$	$A_2 + B_1 + B_2$
A_{2u} A_{1} $A_{1}+A_{2}$ $A_{1}+B_{1}+B_{2}$		$A_1 + B_1 + B_2$
$ \begin{aligned} & E_{u} & A_{1} + A_{2} \\ & T_{lu} & A_{1} + B_{1} + B_{2} \end{aligned} $	A_{1u}	A_2
$T_{lu} A_1 + B_1 + B_2$	A_{2u}	A_1
	E_{u}	$A_1 + A_2$
$T_{2u} \qquad \qquad A_2 + B_1 + B_2$		$A_1 + B_1 + B_2$
	T _{2u}	$A_2 + B_1 + B_2$

Character Table

Дзь	E	2C3	3C2	O_h	253/	30v
A ₁ '	1	1	1	1	1	10
A2'	1	1	-1	1	1	-1
E'	2	-1	0	2) IÇ	0
A1"	1	1	1	-1	143	ŹΠ
A2"	1	1	-1	-1	-1	W 200
Ε"	2	-1	0	-2	1	0707

Oh	E	8C₃	6C2	6C4	3C2	i	6S4	856	3σ _h	6o _d
Aig	1	1	1	1	1	1	1	1	1	1
A _{2g}	1	1	-1	-1	1	1	-1	1	1	-1
E_g	2	-1	0	0	2	2	0	-1	2	0 .
T_{1g}	3	0	-1	1	-1	3	1	0 .	-1	-1
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1
Azu	1	1	1	1	1	-1	-1	-1	-1	-1
A _{2u}	1	1	-1	-1	1	-1	1	-1	-1	1
Eu	2	-1	0	0	2	-2	0	1	-2	0
Tiu	3	0	-1	1	-1	-3	-1	0	1	1
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1

C ₂ v	E	C ₂	$\sigma_{v}(xz)$	$\sigma'_{v}(yz)$
A _I	1	1	1	1
A ₂	1	1	-1	-1
B_1	1	-1	1	-1
B ₂	1	-1	-1	1

試題隨卷繳回