選擇題：每題五選項，每一選項獨立作答。若選項爲正確，用「○」表示。若選項爲不正確，用「✕」表示。例如：每題 (a) ○ (b) ✕ (c) ○ (d) ✕ (e) ✕ 。答對的選項得一分，答錯的選項扣一分，不作答則不計算分數。每題最高可得五分，最低零分。

(1) Which of the following complexes obeys the 18-electron rule (EAN)?
    (a) $[Ni(NH_3)_6]^{2+}$ (b) $Ni(CO)_4$ (c) $[CoCl_4]^{2-}$ (d) $Fe(CO)_5$ (e) $Ni(CN)_4^{2-}$

(2) Which of the following complexes shows a tetrahedral geometry?
    (a) SiH_4 (b) $Ni(CO)_4$ (c) $[CoCl_4]^{2-}$ (d) SF_4 (e) $Ni(CN)_4^{2-}$

(3) Which of the following complexes is paramagnetic?
    (a) $[Ni(NH_3)_6]^{2+}$ (b) $Ni(CO)_4$ (c) $[CoCl_4]^{2-}$ (d) $Fe(CO)_5$ (e) $Ni(CN)_4^{2-}$

(4) Which of the following is a high spin complex?
    (a) $[Ru(NH_3)_6]^{3+}$ (b) $Fe(CN)_6^{4-}$ (c) $Fe(H_2O)_6^{3+}$ (d) $[FeCl_4]^-$ (e) $Co(NH_3)_6^{3+}$

(5) Which of the following octahedral complexes has ^2E ground state?
    (a) d^7 low spin (b) d^5 low spin (c) d^1 (d) d^4 high spin (e) d^9

(6) Which of the following statements describes a typical character for the dissociative mechanism of ligand substitution reactions?
    (a) In a dissociative (D) substitution reaction, loss of a ligand to form an intermediate with a lower coordination number is followed by addition of a new ligand to the intermediate.
    (b) The reaction rate should be strongly dependent on the leaving ligand properties.
    (c) The rate of reaction changes only slightly with changes in the incoming ligand.
    (d) Steric crowding on the reactant complex increases the rate of leaving ligand dissociation.
    (e) Decreasing negative charge or increasing positive charge on the reactant complex usually decreases the rates of substitution.

(7) Two metal carbenes **C** and **D** are shown on the right diagram. Which of the following descriptions about these metal carbenes is incorrect?
    (a) They are called Fischer carbenes.
    (b) In carbene **C**, the W=C bond length is shorter than W-C σ bond.
    (c) Nucleophile tends to undergo attack at the W=C carbon atom of complex **C**.
    (d) Electrophile tends to undergo attack at the Ta=C carbon atom of complex **D**.
    (e) Reaction of C with PhLi would give $(CO)_5W=C(Ph)_2$ as the major product.

(8) Right diagram shows a mechanistic scheme for the Monsanto Process. Four steps labeled respectively as **M, N, O,** and **P** are involved. Which step of the reactions is defined as reductive elimination?

    (a) **M** (b) **N** (c) **O** (d) **P** (e) none
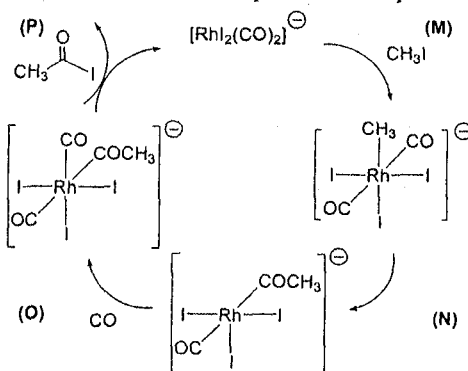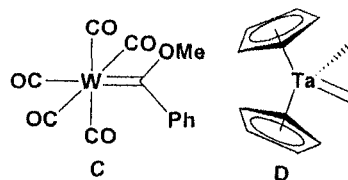
接背面

問答題

I.

(a) Assign the *fac* isomer of $M(CO)_3L_3$ to the proper point group. (1 pts)

fac
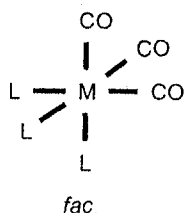
(b) Derive the representation for –CO stretching modes ($\Gamma_{stretch}$) of the *fac* isomer of $M(CO)_3L_3$.　Determine the number and symmetry of –CO stretching modes of the *fac* isomer of $M(CO)_3L_3$.　Which mode is IR active? (4 points)

II.

(a) How many allowed absorption bands would be observed for a d^6 octahedral high spin complex with the Tango-Sugano diagram shown on the right? (1 pts)

(b) Which states are involved in the electronic transition. (1 pts)
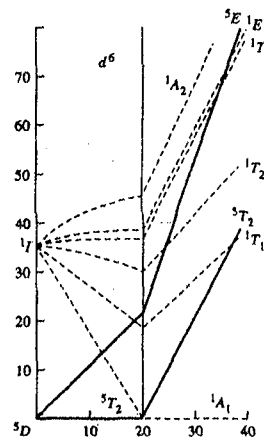
III.

(a) Predict the pKa value for $HClO_4$ according to Pauling's rule.　(1 point)

(b) It has been reported that the pK_1 of H_3PO_3 is 2.00 and the pK_1 of H_3AsO_3 is 9.2.　Predict the Lewis structures of H_3PO_3 and H_3AsO_3 based on their acidity. (2 points)

IV.

(a) Explain briefly the observation that the energy difference between the states of $1s^2 2s^1$ and $1s^2 2p^1$ for Li is 14,904 cm^{-1}, whereas for Li^{2+} the energy difference between the states of $2s^1$ and $2p^1$ is only 2.4 cm^{-1}. (4%)

(b) What are the corresponding spectroscopic notations for these 4 electron configurations? (4%)

V.

Give the symmetry lables for the 3d-, 4s- and 4p-orbitals of the central metal atoms in
(a) $[Cr(en)F_4]^-$, and (b) $[Co(en)_3]^{3+}$. (where "en" is "ethylenediamine") (8%)

VI.

For a **cubic** crystal.

(a) Show the $(12\bar{1})$, (131), and (010) crystal faces. (6%)

(b) What is the angle between (021) and (001) faces? (2%)

VII.

(a) Show the Lewis structure of NO_3^- ion. (2%)

(b) Construct the **π-molecular orbitals and the corresponding energy level diagram** by using "symmetry-adapted linear combination of atomic orbitals". (10%)

(c) FNO_2 is iso-electronic with NO_3^-. What will be the π-MOs and energy levels of FNO_2? (4%)

VIII.

Select the best answer and give the basis for your selection. (10%)

(a)	Most acidic in aqueous solution	HClO	HClO$_2$	HClO$_3$
(b)	Most basic toward BMe_3	Py (pyridine)	2-MePy	4-MePy
(c)	Most basic in aqueous solution	NH$_2$(CH$_3$)	NH(CH$_3$)$_2$	N(CH$_3$)$_3$
(d)	Most acidic toward NH_3	BF$_3$	BCl$_3$	BBr$_3$
(e)	Strongest oxidizing agent	KMnO$_4$	KTcO$_4$	KReO$_4$

接背面

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	

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	1	-1	-1	R_z	
B_1	1	-1	1	1	-1		$x^2 - y^2$
B_2	1	-1	1	-1	1	z	xy
E	2	0	-2	0	0	(x, y); (R_x, R_y)	(xz, yz)

D_{3d}	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$		
A_{1g}	1	1	1	1	1	1		$x^2 + y^2, z^2$
A_{2g}	1	1	-1	1	1	-1	R_z	
E_g	2	-1	0	2	-1	0	(R_x, R_y)	$(x^2 - y^2, xy)$, (xz, yz)
A_{1u}	1	1	1	-1	-1	-1		
A_{2u}	1	1	-1	-1	-1	1	z	
E_u	2	-1	0	-2	1	0	(x, y)	

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2 - x^2 - y^2, x^2 - y^2)$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2(=C_4^2)$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1		
E_g	2	-1	0	0	2	2	0	-1	2	0		$(2z^2 - x^2 - y^2, x^2 - y^2)$
T_{1g}	3	0	-1	1	-1	3	1	0	-1	-1	(R_x, R_y, R_z)	
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1		(xz, yz, xy)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1		
E_u	2	-1	0	0	2	-2	0	1	-2	0		
T_{1u}	3	0	-1	1	-1	-3	-1	0	1	1	(x, y, z)	
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		

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Character Tables

C_1	E
A	1

C_s	E	σ_h		
A'	1	1	x, y, R_z	x^2, y^2, z^2, xy
A''	1	-1	z, R_x, R_y	yz, xz

C_i	E	i		
A_g	1	1	R_x, R_y, R_z	$x^2, y^2, z^2, xy, xz, yz$
A_u	1	-1	x, y, z	

C_2	E	C_2		
A	1	1	z, R_z	x^2, y^2, z^2, xy
B	1	-1	x, y, R_x, R_y	yz, xz

C_3	E	C_3	C_3^2		$\varepsilon = \exp(2\pi i/3)$
A	1	1	1	z, R_z	$x^2 + y^2, z^2$
E	$\begin{Bmatrix}1 \\ 1\end{Bmatrix}$	$\begin{matrix}\varepsilon \\ \varepsilon^*\end{matrix}$	$\begin{matrix}\varepsilon^* \\ \varepsilon\end{matrix}$	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(yz, xz)$

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		x^2, y^2, z^2
B_1	1	1	-1	-1	z, R_z	xy
B_2	1	-1	1	-1	y, R_y	xz
B_3	1	-1	-1	1	x, R_x	yz

D_3	E	$2C_3$	$3C_2$		
A_1	1	1	1		$x^2 + y^2, z^2$
A_2	1	1	-1	z, R_z	
E	2	-1	0	$(x, y)(R_x, R_y)$	$(x^2 - y^2, xy)(xz, yz)$

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

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

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x, R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x, y	

C_{3h}	E	C_3	C_3^2	σ_h	S_3	S_3^5		$\varepsilon = \exp(2\pi i/3)$
A'	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
E'	$\begin{Bmatrix}1 \\ 1\end{Bmatrix}$	$\begin{matrix}\varepsilon \\ \varepsilon^*\end{matrix}$	$\begin{matrix}\varepsilon^* \\ \varepsilon\end{matrix}$	$\begin{matrix}1 \\ 1\end{matrix}$	$\begin{matrix}\varepsilon \\ \varepsilon^*\end{matrix}$	$\begin{matrix}\varepsilon^* \\ \varepsilon\end{matrix}$	(x, y)	$(x^2 - y^2, xy)$
A''	1	1	1	-1	-1	-1	z	
E''	$\begin{Bmatrix}1 \\ 1\end{Bmatrix}$	$\begin{matrix}\varepsilon \\ \varepsilon^*\end{matrix}$	$\begin{matrix}\varepsilon^* \\ \varepsilon\end{matrix}$	$\begin{matrix}-1 \\ -1\end{matrix}$	$\begin{matrix}-\varepsilon \\ -\varepsilon^*\end{matrix}$	$\begin{matrix}-\varepsilon^* \\ -\varepsilon\end{matrix}$	(R_x, R_y)	(xz, yz)

試題隨卷繳回