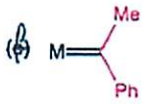
① (eg) M—NR_3 amine 2 e⁻

(a) M—NR_2 (b) M=NR (c) M≡N (d) M=O (e) 

(f)  (g) M—PR_2 (h) M—H (i) M—CO (j) M—≡N—R

a) Amide 2e⁻

b) Imide 4e⁻

c) Nitride 6e⁻

d) Oxo 4e⁻

e) Allyl 4e⁻

f) Carbene 4e⁻

g) Phosphide 4e⁻

h) Hydride 2e⁻

i) Carbonyl 2e⁻

j) Isonitrile 2e⁻

② a) Co^{1-}, d^{10}

↿⇂ ↿⇂ ↿⇂

↿⇂ ↿⇂

CFSE = 0

b) Cr^{2+}, d^4

— —

↿⇂ 1 1

CFSE = $1.6\Delta_o - P$

c) Fe^{3+}, d^5

— —

↿⇂ ↿⇂ 1

CFSE = $2\Delta_o - 2P$

d) Fe^{3+}, d^5

1 1

1 1 1

CFSE = 0

e) Co^{2+}, d^7

1 1

↿⇂ ↿⇂ 1

CFSE = $0.8\Delta_o - 2P$

f) Co^{3+}, d^6

— —

↿⇂ ↿⇂ ↿⇂

CFSE = $2.4\Delta_o - 3P$

g) Mn^{7+}, d^0

— — —

— —

CFSE = 0

h) Cu^{2+}, d^9

↿⇂ 1

↿⇂ ↿⇂ ↿⇂

CFSE = $0.6\Delta_o - 4P$

i) Ru^{2+}, d^6

— —

↿⇂ ↿⇂ ↿⇂

CFSE = $2.4\Delta_o - 3P$

j) Fe^{3+}, d^5

1 1 1

1 1

CFSE = 0

(3) Consider a d^2 transition metal ion such as Ti^{2+}.

(a) There are five terms that describe the 45 microstates for a d^2 ion. These terms are ^1S, ^1D, ^1G, ^3P and ^3F. Which of these terms is the ground state term for a d^2 system? (5 pts)

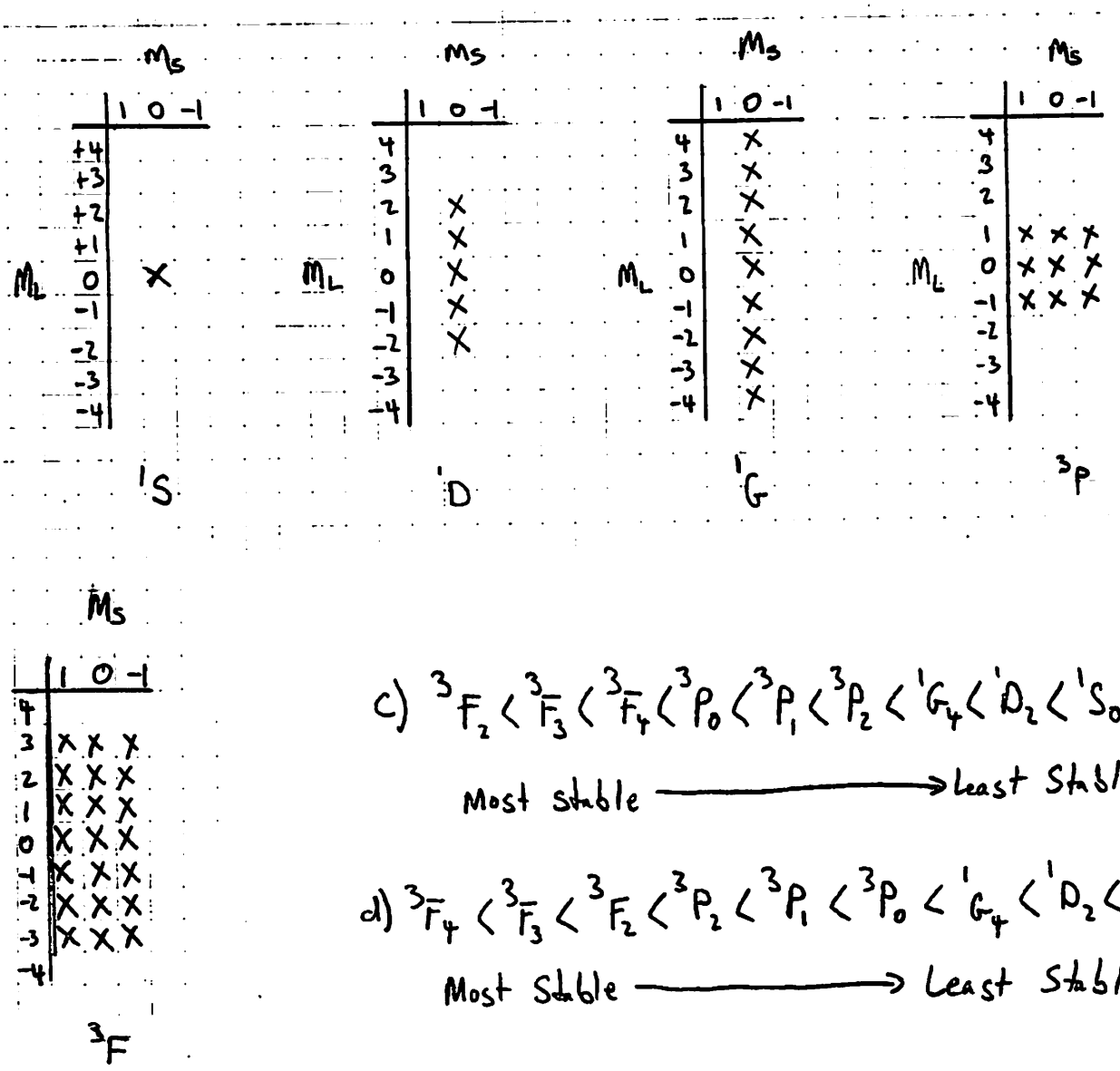
(b) Construct a microstate table for each of the term symbols listed in part (a) and show which collection of microstates belongs to each one. (15 pts)

(c) Consider how spin orbit coupling will split each of these terms into states of different energy. Derive all of the states that arise from L—S coupling for each term and order them in terms of stability. (10 pts)

(d) The term symbols for a d^8 metal ion such as Ni^{2+} are the same as for the d^2 case. How would you order each of the states arising from L—S coupling for this metal ion? (10 points)

a) ^3F ⟶ Highest Multiplicity + value of L

b)



c) $^3F_2 < {}^3F_3 < {}^3F_4 < {}^3P_0 < {}^3P_1 < {}^3P_2 < {}^1G_4 < {}^1D_2 < {}^1S_0$

Most stable ⟶ Least Stable

d) $^3F_4 < {}^3F_3 < {}^3F_2 < {}^3P_2 < {}^3P_1 < {}^3P_0 < {}^1G_4 < {}^1D_2 < {}^1S_0$

Most Stable ⟶ Least Stable

(4) Consider the Tanabe-Sugano diagram for the d^5 electron configuration (http://en.wikipedia.org/wiki/Tanabe-Sugano_diagram) in answering the following. (15 pts)

(a) What is the term symbol for the ground state of a free d^5 ion where $\Delta_o/B = 0$? (3 pts)

^6S

(b) What is the term symbol for the ground state of a free d^5 ion where $\Delta_o/B = 20$? (3 pts)

$^6A_1$

(c) What is the physical meaning of the discontinuity in the TS-diagram around $\Delta_o/B = 28$? (3 pts)

Represents the transition from High Spin (weak field) to Low Spin (Strong Field)

(d) How many spin allowed transitions are expected for the d^5 case for $\Delta_o/B < 28$? (3 pts)

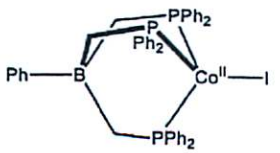
0

(e) How many spin allowed transitions are expected for the d^5 case for $\Delta_o/B > 28$? (3 pts)

4

(5) Using the Tanabe-Sugano diagrams found at http://en.wikipedia.org/wiki/Tanabe-Sugano_diagram, determine how many absorption transitions are expected for each of the complexes below. (20 pts)

(a) $[Cr(CN)_6]^{4-}$ – 4
(b) $[Cr(H_2O)_6]^{2+}$ – 1
(c) $[TiF_6]^{2-}$ – 0
(d) $[Ti(OH_2)_6]^{3+}$ – 1
(e) $[MnF_6]^{4-}$ – 0
(f) $V(CO)_6$ – 4
(g) $[Ru(bpy)_3]^{2+}$ – 5
(h) $[Tc(CN\text{-}tBu)_6]^{+}$ – 5
(i) $[Co(NH_3)_6]^{2+}$ – 3
(j)



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