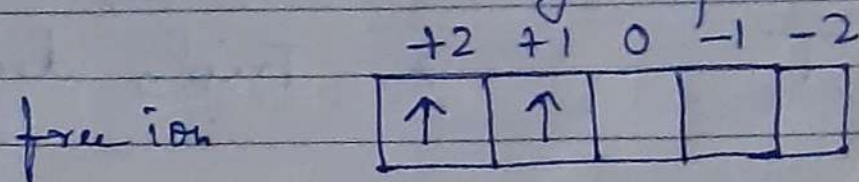


# ORAEEL Diagram (F term):-

$d^2 \rightarrow$  octahedral high spin



$L = 2+1=3$  , F term

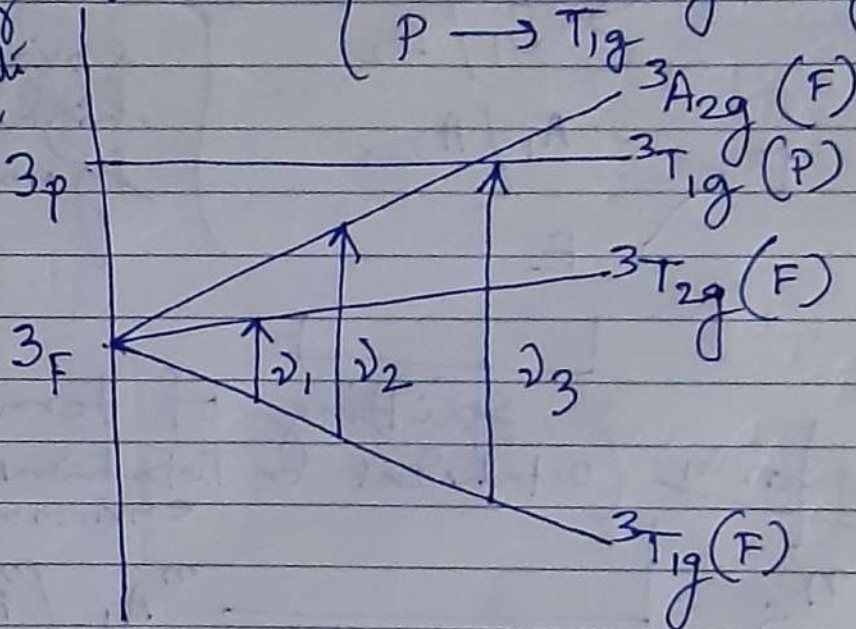
$S = \frac{1}{2} + \frac{1}{2} = 1$  ,  $2S+1 = 3$

Ground State Term  $3F$

for octahedral cases

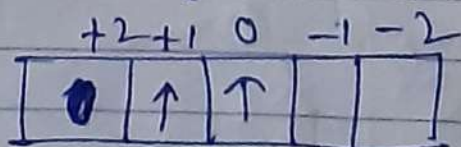
$F \rightarrow A_{2g}, T_{2g}, T_{1g}$   
 $P \rightarrow T_{1g}$

(We are excluding other excited states here as the other transitions are very less intense)



$\rightarrow Dq$   
 Increasing ligand field

\* How  $(3P)$  is generated?



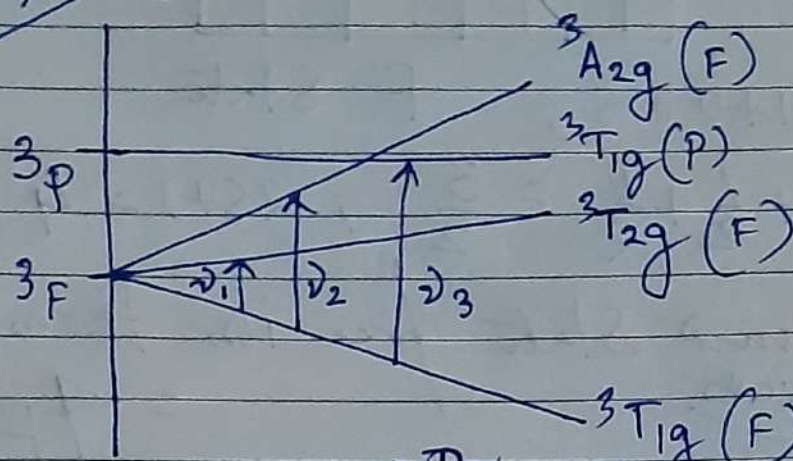
$L = 1$  , P State

$S = \frac{1}{2} + \frac{1}{2} = 1$  ,  $2S+1 = 3$



# Case Studies :-

## Case I (Common)



${}^3T_{1g}(F)$  = Ground state

${}^3T_{2g}(F)$  = First excited state

Increasing ligand field  $\Delta_o$

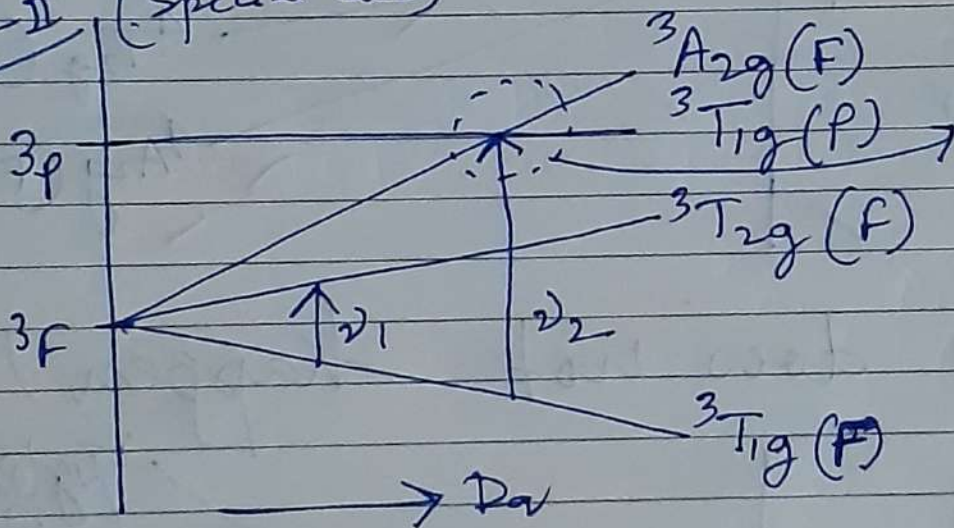
$\nu_1 \Rightarrow {}^3T_{1g}(F) \rightarrow {}^3T_{2g}(F)$

$\nu_2 \Rightarrow {}^3T_{1g}(F) \rightarrow {}^3A_{2g}(F)$

$\nu_3 \Rightarrow {}^3T_{1g}(F) \rightarrow {}^3T_{1g}(P)$

Three bands are expected

## Case II (Special case)



Cross over region

${}^3T_{1g}(F) \rightarrow$  Ground state

${}^3T_{2g}(F)$  = 1st excited state (ES)

In a particular ligand environment

$\nu_1 \Rightarrow {}^3T_{1g}(F) \rightarrow {}^3T_{2g}(F)$

$\nu_2 \Rightarrow {}^3T_{1g}(F) \rightarrow {}^3T_{1g}(P)/{}^3A_{2g}(F)$

Crossover region

Two bands is expected and one missing band is observed.



# $d^3$ octahedral high spin

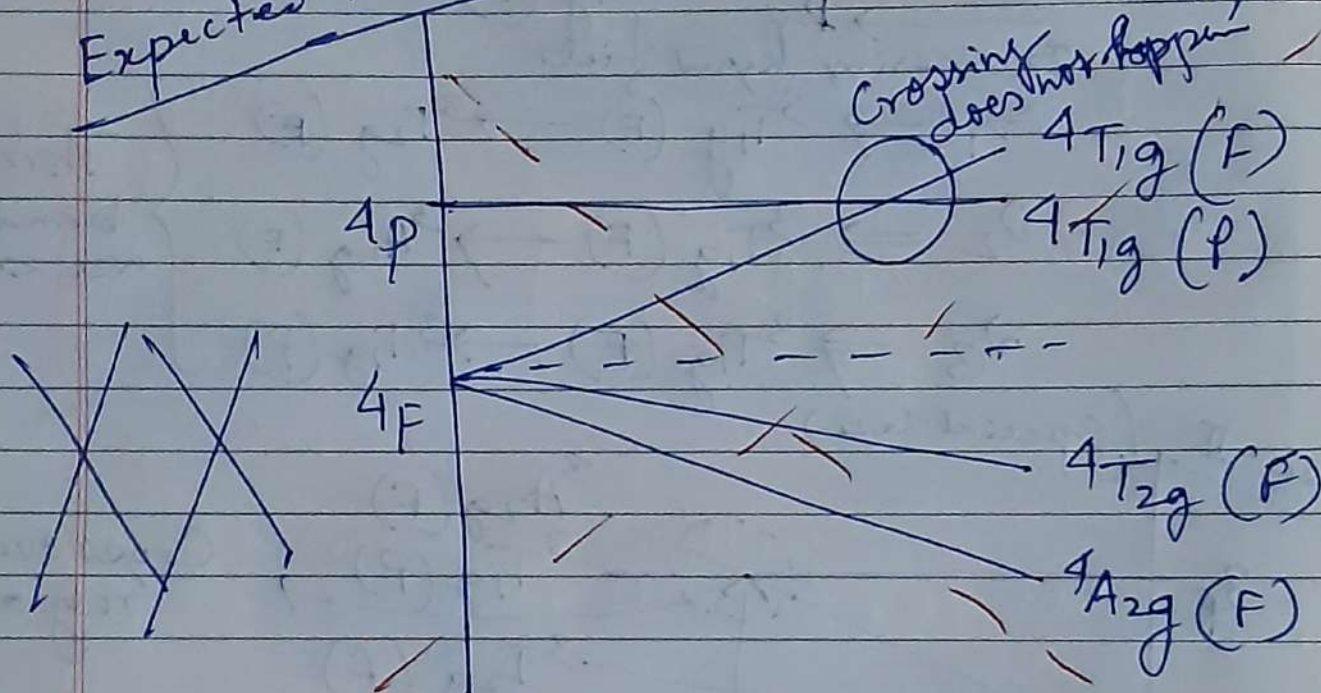
+2	+1	0	-1	-2
↑	↑	↑		

$$L = 2 + 1 + 0 = 3, \quad F \text{ State}$$

$$S = \frac{1}{2} + \frac{1}{2} + \frac{1}{2} = \frac{3}{2}, \quad 2S+1 = 4$$

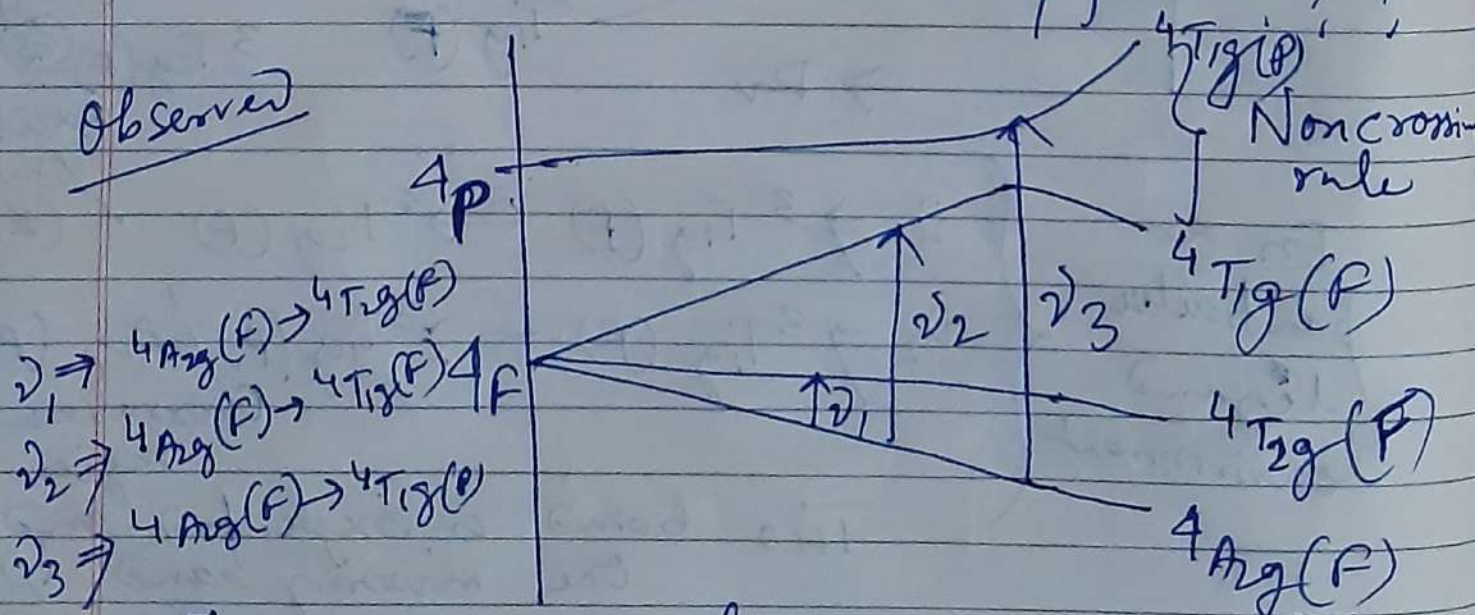
Ground State free ion term =  $4F$

Expected theoretically



It does not happen!!!

Observed



Three peaks are observed.



Related Topic :- (It is expected that Students are aware about CFT very well)

- \* (1) How  $v_1, v_2, v_3$  can be calculated?
- (2) What is Racah parameter?
- \* (3) What is non crossing rule?
- \* (4) How  $A_{1g}, T_{1g}$  terms are generated from  $S, P, D, F$  free ion term?
- (5) How  $\Delta_o$  and  $\Delta_t$  value can be calculated from ORGEL diagram?
- \* (6) What is the energy difference between  $n_F \rightarrow n_P$  (Free ions)
- (7) ORGEL diagram shows good result in weak field ligand.
- (8) Tetrahedral Complexes are high spin Complex. Why?
- \* (9) Construct the other higher terms for  $d^2$  and  $d^3$  system.