

Tanabe Sugano (TS) Diagram

Lecture - 2

M. Sc. (CC-6/PAT/CSIR NET)
Inorganic Chemistry

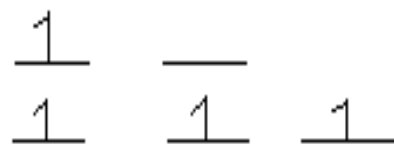
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For d⁴ system

d⁴ is field dependent system i.e. its splitting depends upon W/F & S/F

Weak field



$$M_s = 2 \times \frac{4}{2} + 1 = 5$$

$$L = +2 + 1 + 0 - 1$$

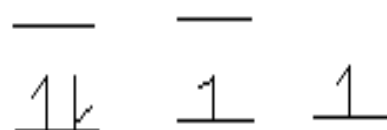
$$= 2 \quad (0, 1, 2 \Rightarrow S, P, D)$$

So, G.S.T = ⁵D

⁵D splits into ⁵E_g & ⁵T_{2g}

Since E_g set is incomplete so ⁵E_g
is ground state is degeneracy

Strong Field



$$d^4 = d^3 + d^1$$

$$2 \times \frac{2}{2} + 1 = 3$$

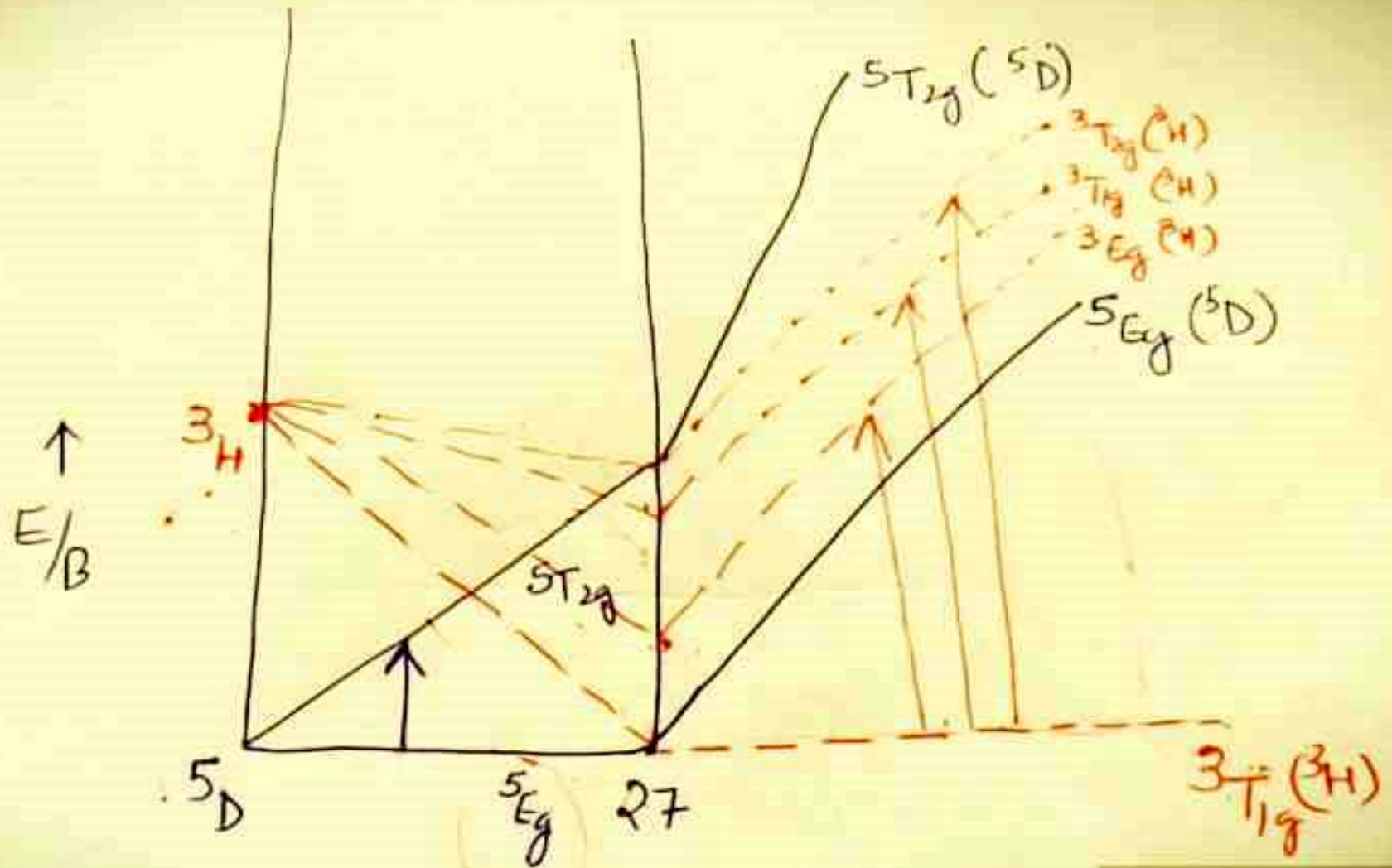
$$L = +2 + 2 + 1 + 0 = 5 \quad (0, 1, 2, 3, 4, 5 \Rightarrow S, P, D, F, G, H)$$

Since J=L+S for more than half filled orbital. So G.S.T. = ³H

³H, (³G, ³F, ³D, ³P, ¹I, ¹G, ¹F, ¹D, ¹S)

³H splits into ³E_g, ³T_{1g}, ³T_{1g}, ³T_{2g}

T_{2g} term is incomplete so G.S. degeneracy
is A_{1g} X T_{2g} = ³T_{1g}

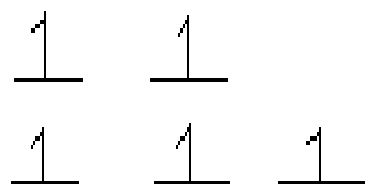


In weak field there is only one peak due to transition of electron from $^5E_{2g}$ to $^5T_{2g}$ followed by spin allowed transition ($\Delta S=0$). But in strong field there are 3 peaks are obtained due to spin allowed transition of electron.

TS diagram of d^5 system

d^5 is field dependent system i.e. its splitting depends upon W/F & S/F

Weak field

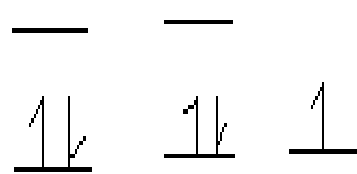


$$M_s = 2 \times \frac{5}{2} + 1 = 6$$

$$L = 0 \text{ (S)}$$

$$\text{So, G.S.T} = {}^6S \Rightarrow {}^6A_{1g}$$

Strong Field



$$d^3X d^2 = A_{2g}XT_{1g} = T_{2g}$$

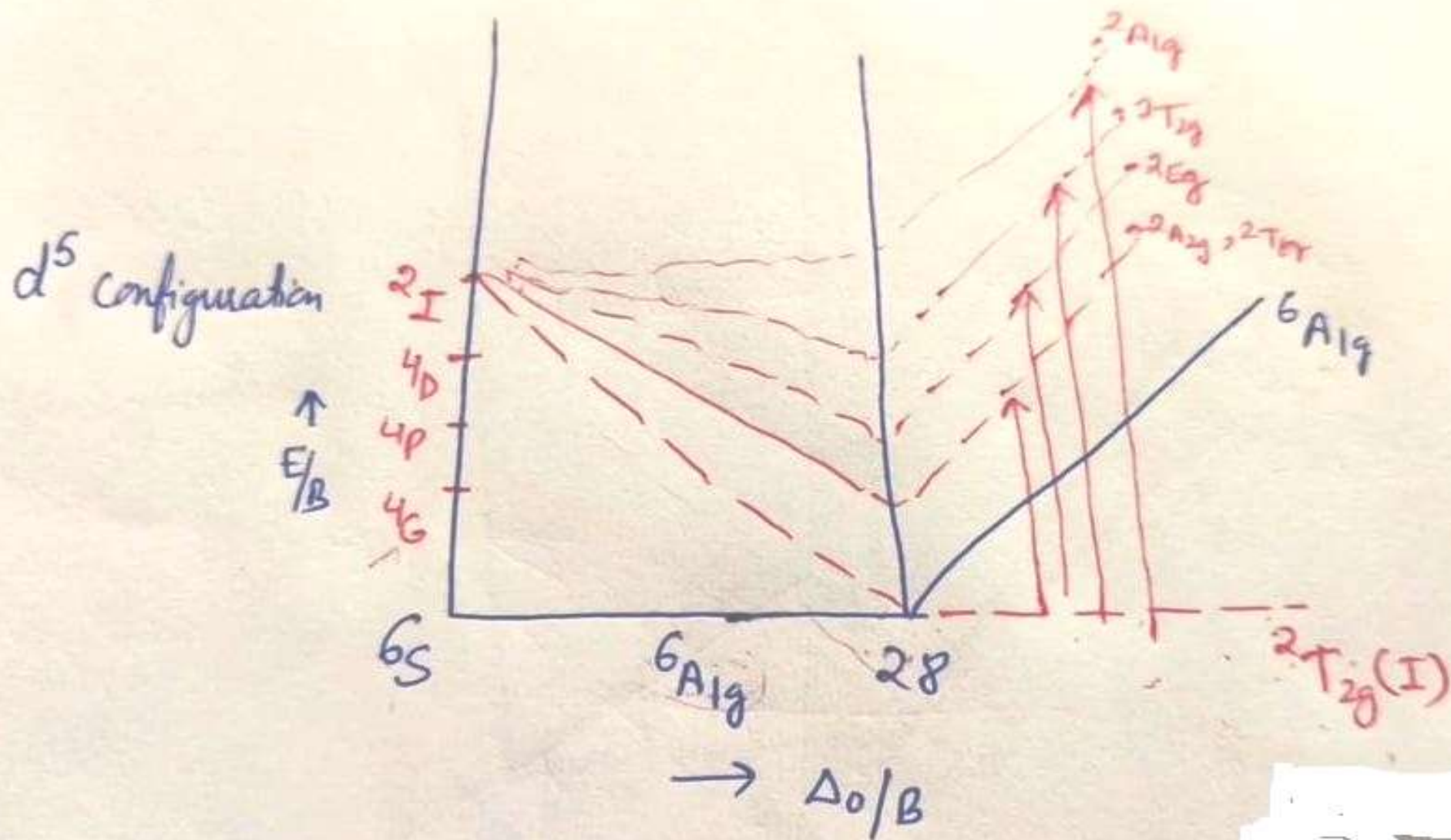
$$2 \times \frac{1}{2} + 1 = 2$$

$$L = +2+2+1+1+0 = 6 \text{ (0, 1, 2, 3, 4, 5} \Rightarrow \text{S, P, D, F, G, H, I)}$$

So, terms will be ${}^1I, {}^2H, {}^2G, {}^2F, {}^2D, {}^2P, {}^2S$

Since T_{2g} set is incomplete. So ground degenerated term is T_{2g}

So, TS diagram may be sketched as in both W/F & S/F

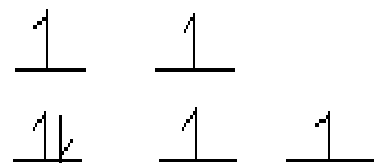


In weak field no peak is obtained but in strong field we get for spin allowed peaks where $\Delta s = 0$

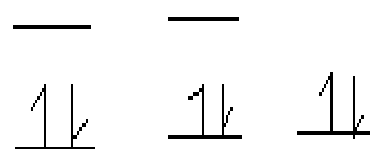
TS diagram of d^6 system

d^6 is field dependent system i.e. its splitting depends upon W/F & S/F

Weak field



Strong Field



$$M_s = 2 \times \frac{4}{2} + 1 = 5$$

$$2 \times \frac{0}{2} + 1 = 1$$

$$L = +2 + 2 + 1 + 1 + 0 + 0 = 6 \quad (0, 1, 2) = S, P, D$$

$$L = +2 + 2 + 1 + 1 + 0 + 0 = 6 \quad (0, 1, 2, 3, 4, 5 \Rightarrow S, P, D, F, G, H, I)$$

$$\text{Terms energy} = {}^1I < {}^1H < {}^1G < {}^1F < {}^1D < {}^1P < {}^1S$$

$$\text{So, G.S.T} = {}^5D < {}^6P < {}^6S$$

$${}^1I \text{ splits into } A_{1g} + A_{2g} + E_g + T_{1g} + {}^2T_{2g}$$

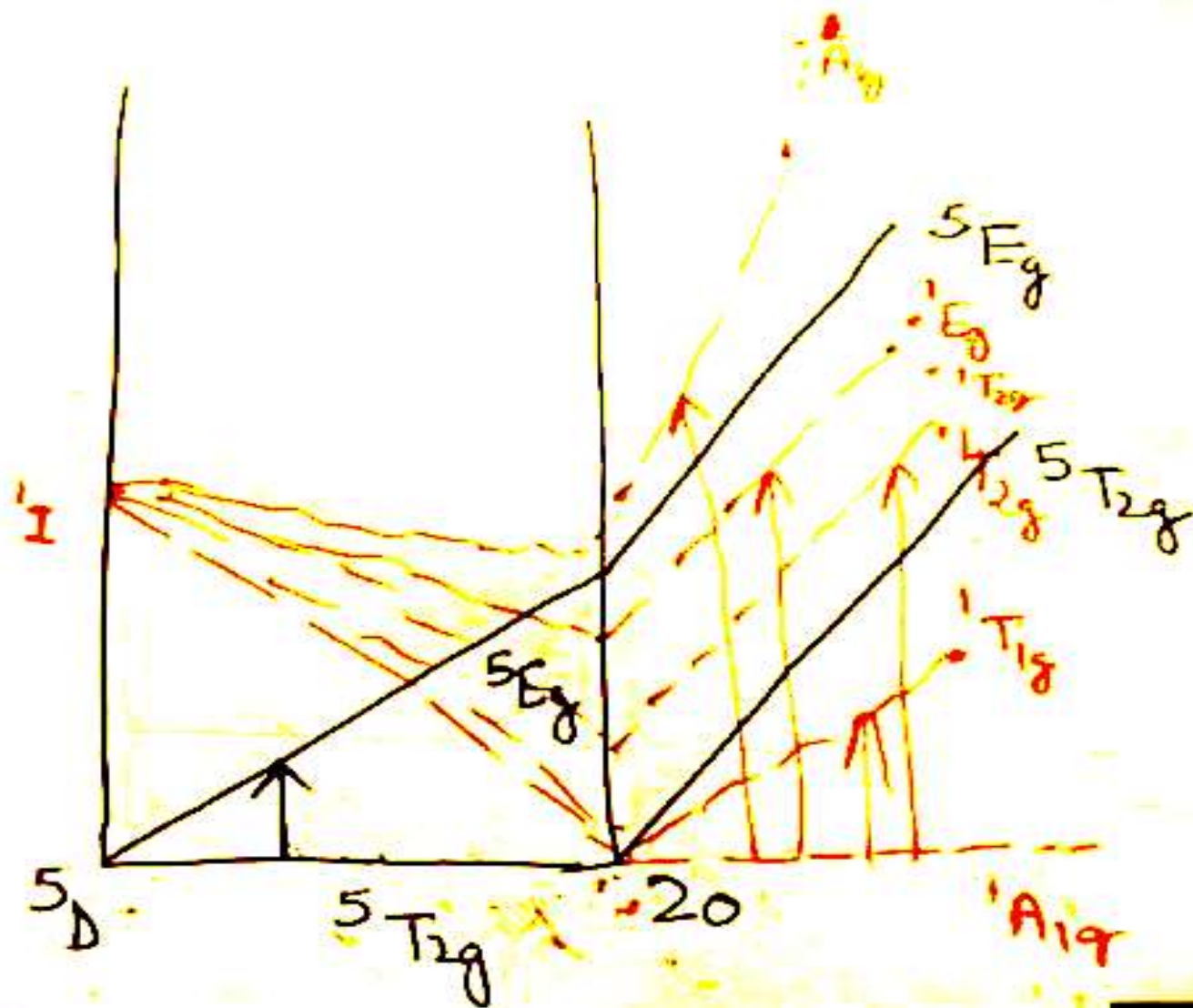
$${}^5D \text{ splits into } {}^5T_{2g}, {}^5E_g \text{ but } T_{2g} \text{ is incomplete}$$

$$\text{So, G.S.T. degeneracy is } {}^5T_{2g}$$

So, TS diagram may be sketched as in both W/F & S/F

d^6
Configuration

\uparrow
 E/B

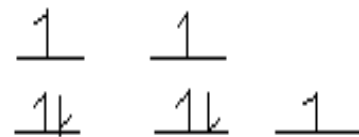


We get only one peak in weak field & four peaks in strong field as given in diagram.

TS diagram of d^7 system

d^7 is field dependent system i.e. its splitting depends upon W/F & S/F

Weak field



$$M_s = 2 \times \frac{3}{2} + 1 = 4$$

$$L = +2 + 2 + 1 + 1 + 0 + 0 - 1 = 5 \quad (0, 1, 2, 3) = S, P, D, F$$

$$G.S.T. = {}^4F$$

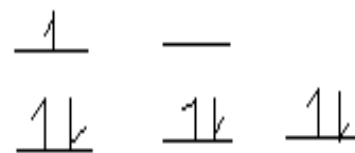
$$\text{Energy of terms} = {}^4F, {}^4D < {}^4P < {}^4S$$

4F splits into ${}^1T_{1g}$, ${}^4T_{1g}$ & ${}^4A_{2g}$

but T_{2g} is incomplete

So G.S.T degeneracy is ${}^4T_{1g}$

Strong Field



$$2 \times \frac{1}{2} + 1 = 2$$

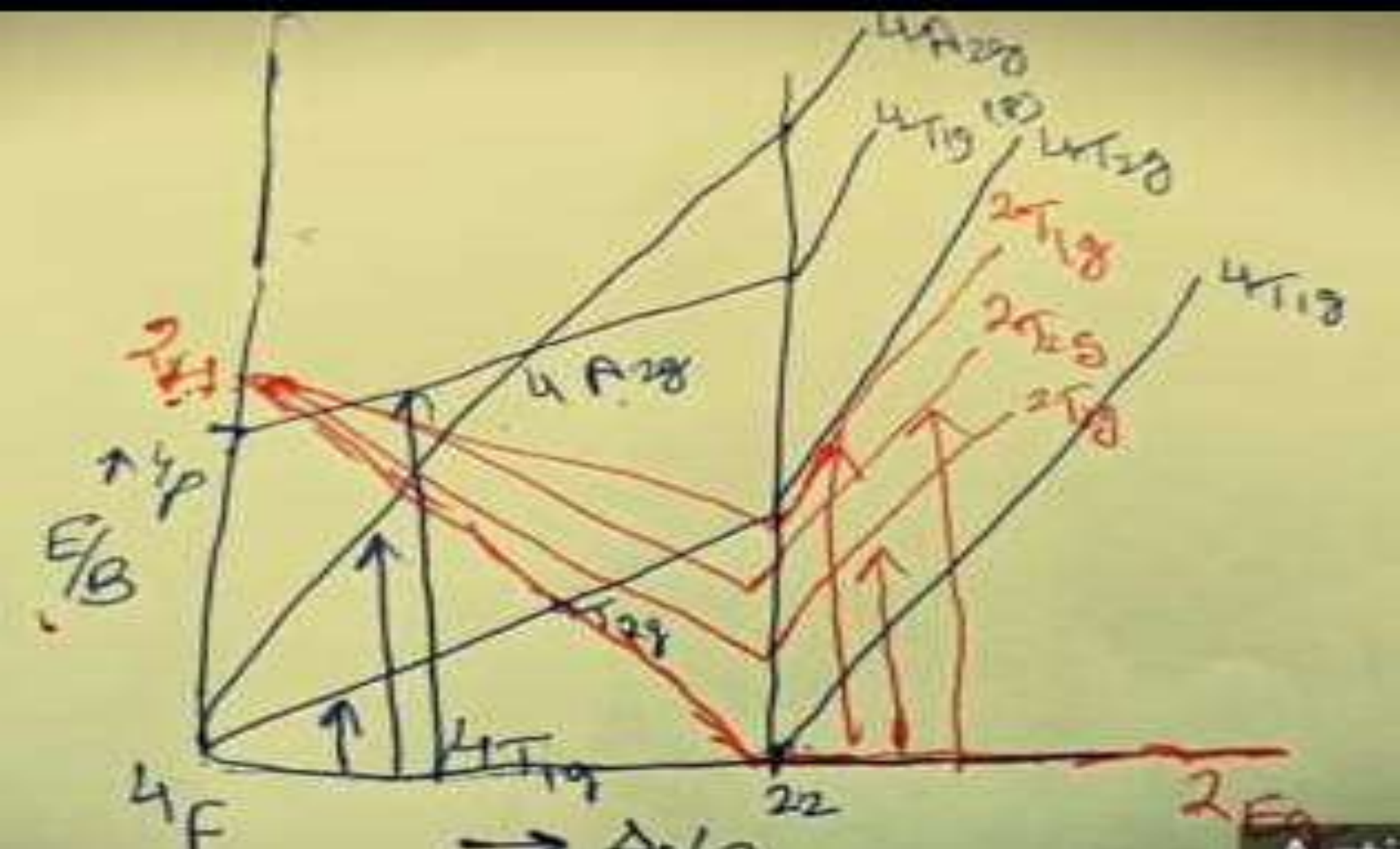
$$L = +2 + 2 + 1 + 1 + 0 + 0 - 1 = 5 \quad (0, 1, 2, 3, 4, 5 \Rightarrow S, P, D, F, G, H)$$

$$\text{Terms energy} = {}^2H < {}^2G < {}^2F < {}^2D < {}^2P < {}^2S$$

2H splits into ${}^2E_g + {}^2T_{1g} + {}^2T_{2g} + {}^2T_{2g}$

E_g is incomplete So G.S.T generated is 2E_g

So, TS diagram may be sketched as in both W/F & S/F



There are 3 peaks in weak field & 3 peaks in strong field are obtained due to electronic transfer in d^7 system.



Thank You

