Tanabe Sugano (TS) Diagram
Lecture-1

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

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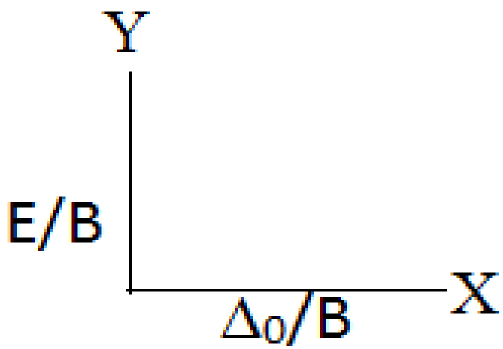
Tanabe Sugano (TS) Diagram

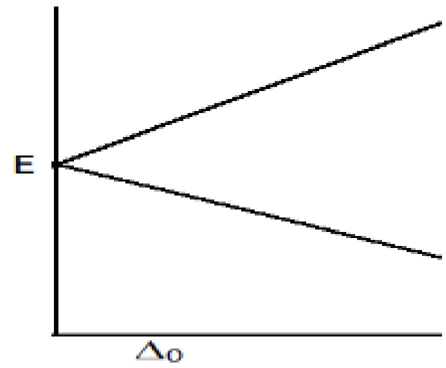
(It was Proposed by Yukito Tanabe & Satoru Sugano in 1954 on the absorption of spectra of complexes published in a journal).

Splitting of terms in strong field (as well as weak field) is called TS diagram.

It gives idea about e-spectra & is more comprehensive then orgel diagram. It is just like orgel diagram except.

1. It is plotted b/w ligand field strength (Δ_0/B) & excited state term (E/B) along X axis & Y axis respectively. (Where B = Racah Parameter which play important role in TS diagram, Δ_0 = CFSE, E = energy of term) unlike orgel diagram.

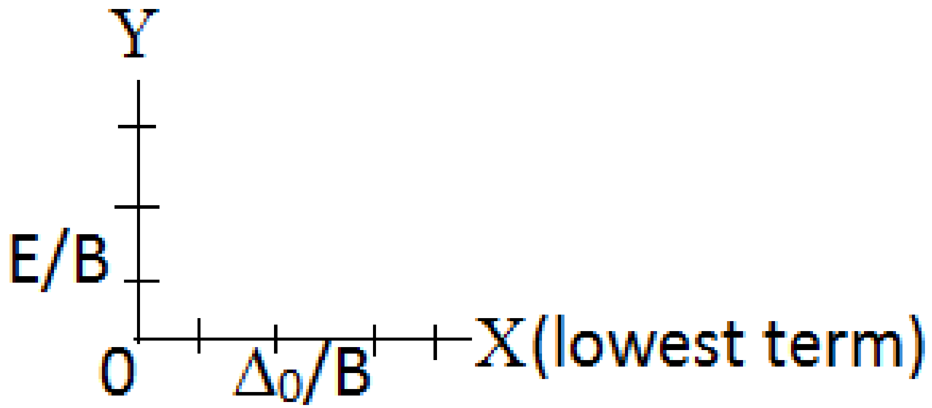




TS Diagram

Orgel Diagram

2. Ground State is taken as constant reference & energy is zero than other splitted terms



3. It is valid for both HS & LS (weak field & strong field) &follow non crossing rule.

4. All terms of different microstates are considered in TS diagram even forbidden transition occurs unlike orgel diagram.

5. It helps to calculate Δ_0, B, ß (Nephlauxetic ratio).

To sketch TS diagram microstates, possible terms, GST & their stability (energy) & orgel diagram must be considered

$$\text{No. of Microstate} = \frac{\lfloor n}{\lfloor e \ \lfloor n-e}$$

n = twice of the no. of orientation of orbital

e = No. of given e-

Microstates for nd^{1-10}

configuration	d^1	d^2	d^3	d^4	d^5	d^6	d^7	d^8	d^9	d^{10}
microstates	10	45	120	210	252	210	120	45	10	1

The number of microstates (the total degeneracy) for a configuration nd^x is the same as for nd^{10-x}.

configuration	atomic terms
d^1, d^9	^2D
d^2, d^8	^3F, ^3P, ^1G, ^1D, ^1S
d^3, d^7	^4F, ^4P, ^2H, ^2G, ^2F, ^2D
d^4, d^6	^5D, ^3H, ^3G, ^3F, ^3D, ^3P, ^1I, ^1G, ^1F, ^1D, ^1S
d^5	^6S, ^4G, ^4F, ^4D, ^4P, ^2I, ^2H, ^2G, $^2G'$, ^2F, $^2F'$, ^2D, $^2D'$, ^2P, ^2S
d^{10}	^1S

1. Term with highest spin multiplicity 2S+1 has lowest energy.
2. Terms with same multiplicity, that one with highest value of L is lower in energy (S < P < D < F < G < H < I)

e.g. $^3F < {}^3P$ - for d^2, d^8,

$^4F < {}^4P$ - for d^3, d^7

Splitting of term

L	Term	Term splitting in octahedral field
0	S	A_{1g}
1	P	T_{1g}
2	D	$E_g + T_{2g}$
3	F	$A_{2g} + T_{1g} + T_{2g}$
4	G	$A_{1g} + E_g + T_{1g} + T_{2g}$
5	H	$E_g + {}^2T_{1g} + T_{2g}$
6	I	$A_{1g} + A_{2g} + E_g + T_{1g} + T_{2g} + T_{2g}$

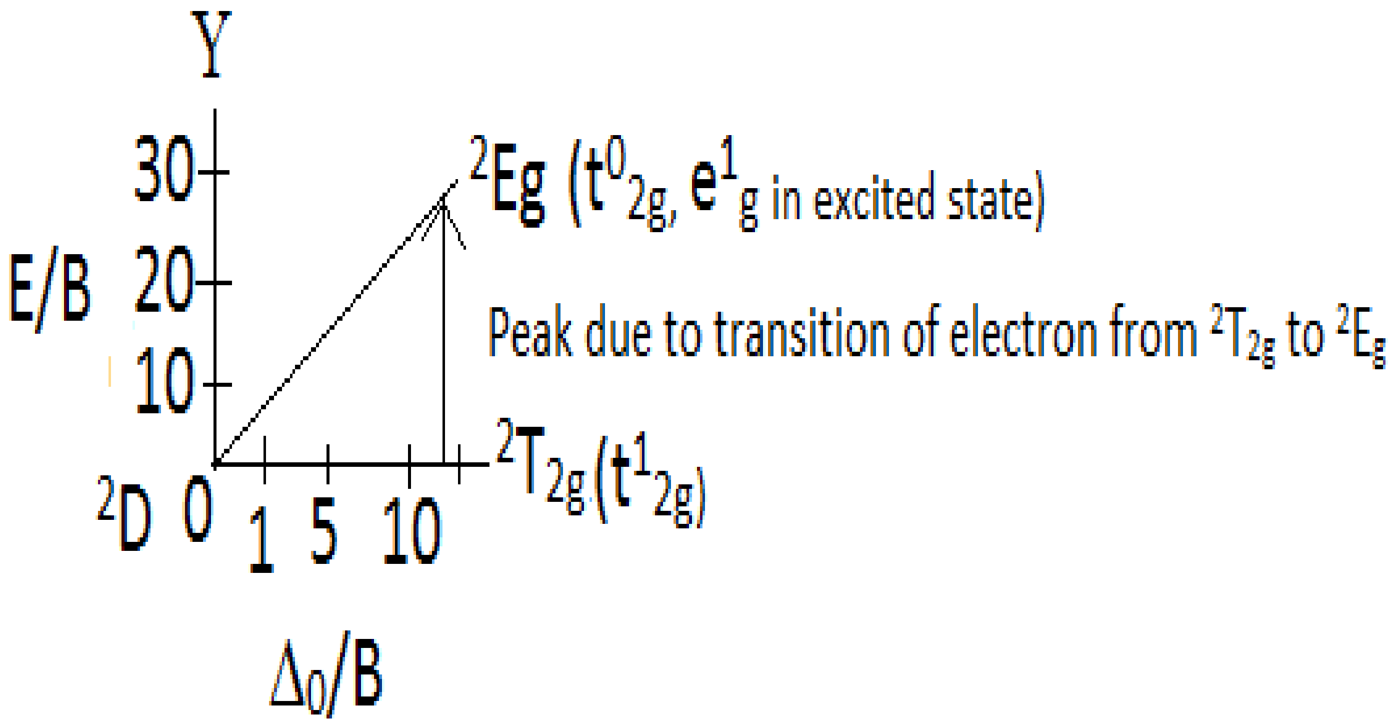
d^1, d^2, d^3, d^8, d^9 & d^{10} are field independent system so there is no change in weak or strong field but d^4, d^5, d^6 & d^7 are field dependent system. So there is change in spectral peak of weak field & strong field complexes.

Now we discuss about TS diagram of d^n system.

For d^1 & d^9 system

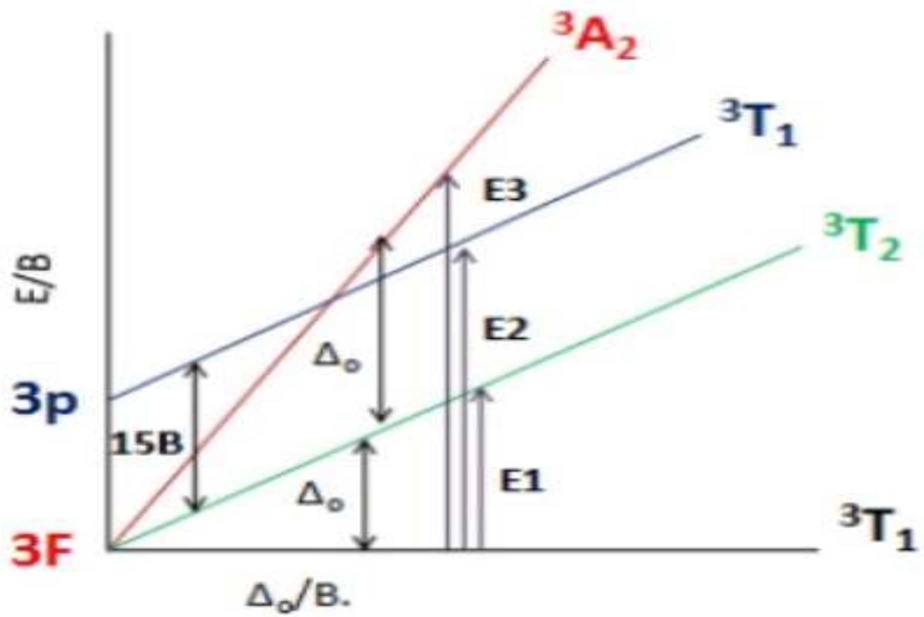
Microstates of d^1 & d^9 system is ^2D

^2D splits into two sets t^1_{2g} & e^1_g where $^2T_{2g}$ has lowest energy & goes to X axis



For d^2 system

Ground states term of d^2 & d^8 system are ^3F, ^3P, ^1G, ^1D, ^1S but stable terms are ^3F & ^3P where energy of $^3F < ^3P$



As we know that energy difference b/w two terms of same multiplicity (^3F & ^3P) = 15B & we get 3 transition peaks E1, E2, E3 (however other transition are also b/w different terms are possible but they are not allowed)

Example: $[V(H_2O)_6]^{3+}$

Thank You