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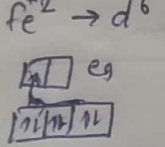
Orgel diagrams (inter electronic interaction)

Orgel Diagrams are correlation diagrams which show the relative energies of electronic terms in transition metal complexes. They are named after their creator Leslie Orgel.

* Orgel diagrams are used for interpretation of spin allowed absorption bands of d-d origin in the electronic Spectra of tetrahedral and octahedral transition metal complexes.
* It is used to assign the electronic transition in weak field or high Spin transition metal complex and all tetrahedral complex.
* It cannot be used for low spin or strong field complexes. because Octahedral field is stronger than d-d inter electronic repulsion.

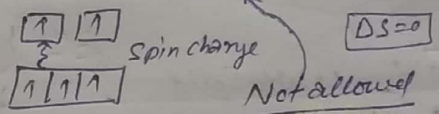
$\Rightarrow [Fe(CN)_6]^{-4}$

$Fe^{+2} \rightarrow d^6$ [L.S] allowed transition



$\Rightarrow [Mn(H_2O)_6]^{+2}$

$Mn^{+2} \rightarrow d^5$ [H.S]



Mulliken term Symbol →

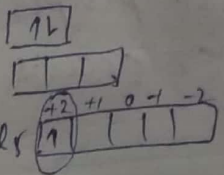
Mulliken term Symbol	octahedral filled (Oh)	Tetrahedral filled (Td)
S	A_{1g}	A_1
P	T_{1g}	T_1
D	$T_{2g} + E_g$	$T_2 + E$
F	$T_{1g} + T_{2g} + A_{2g}$	$T_1 + T_2 + A_2$
G	$T_{1g} + T_{2g} + E_g + A_{1g}$	$T_1 + T_2 + E + A_1$
H	$2T_{1g} + T_{2g} + E_g$	$2T_1 + T_2 + E$
I	$2T_{2g} + T_{1g} + E_g + A_{1g} + A_{2g}$	$2T_2 + T_1 + E + A_1 + A_2$

S = 0 $l_1 + l = 0$

P = 1 $l_1 + l_2 + l_3 = 1$

d = 2 $l_1 + l_2 + l_3 + l_4 + l_5$

F = 3

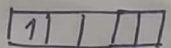


configuration	Energy term	Ground state & Excited state Term of Same multiplicity
d^1, d^9	^2D	$^2T_{2g}$, ^2E_g
d^2, d^8	^3P	$^3T_{1g}(P)$
	^3F	$^3T_{1g(F)}$, $^3T_{2g}$ $^3A_{2g}$
d^3 d^7	^4P	$^4T_{1g}(P)$
	^4F	$^4T_{1g(F)}$ $^4T_{2g}$ $^4A_{2g}$
d^4 d^6	^5D	$^5T_{2g}$ ^5E_g

d^1 System - $[Ti(H_2O)_6]^{+3}$

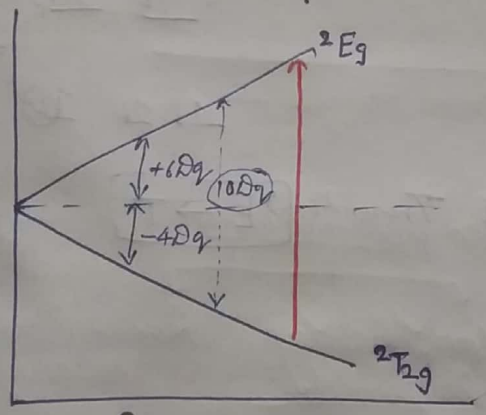
$_{22}Ti = [Ar]\ 3d^2, 4s^2$

$Ti^{+3} = [Ar], 3d^1$ The G.S term for d^1 Sys is



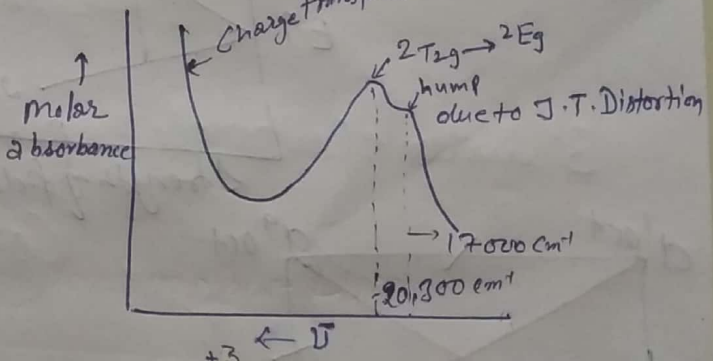
$2S+1 = 2\times\frac{1}{2}+1 = 2$ ^2D

⇒ ^2D Splits in Octahedral Field Complex as —



$^2E_g + {}^2T_{2g}$

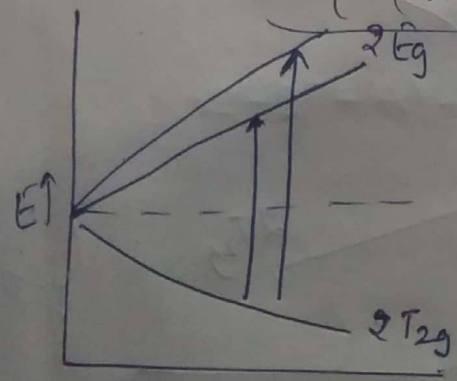
Spectrum ⇒



$[Ti(H_2O)_6]^{+3}$

Que ⇒ If $[Ti(H_2O)_6]^{+3} = 20,000\ cm^{-1}$ then find the value of CFSE (H.W) ↪ $4D_q$

Ans ⇒ $[Ti(H_2O)_6]^{+3}$ has d^1 system.

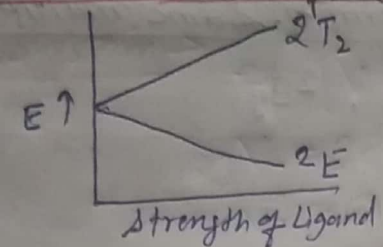


$\therefore 10D_q = 20000\ cm^{-1}$

$4D_q = \frac{20,000}{10} \times 4 = 8000\ cm^{-1}$

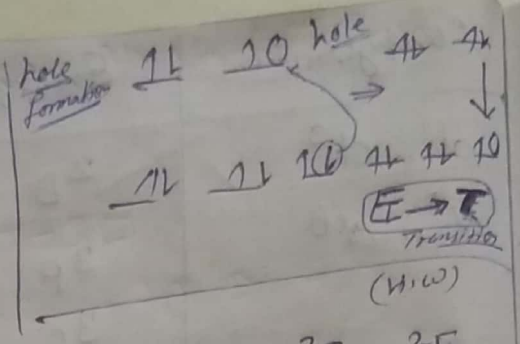
Splitting takes place due to John-Teller distortion (As gives 2 peaks)

In tetrahedral field →



(H.W)

$^2T_2 \leftarrow {}^2E$

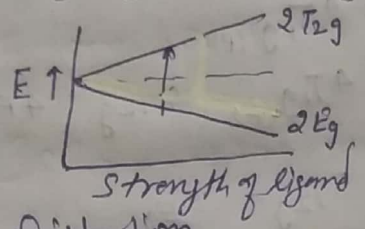


d^9 System → eg → $[Cu(H_2O)_6]^{+2}$

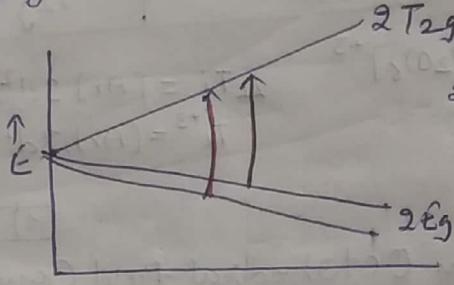
(oh)

G.S Term = $^2D \rightarrow {}^2T_{2g} + {}^2E_g$.

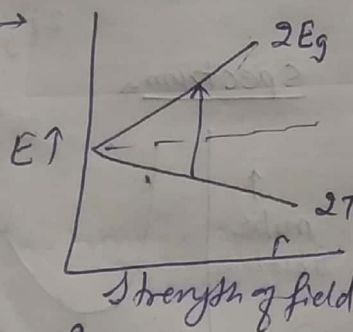
$Cu^{+2} = d^9$

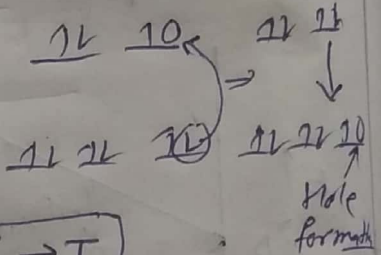


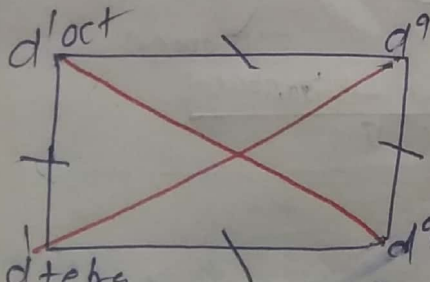
∴ due to J-T. Distortion



d^9 tetrahedral →

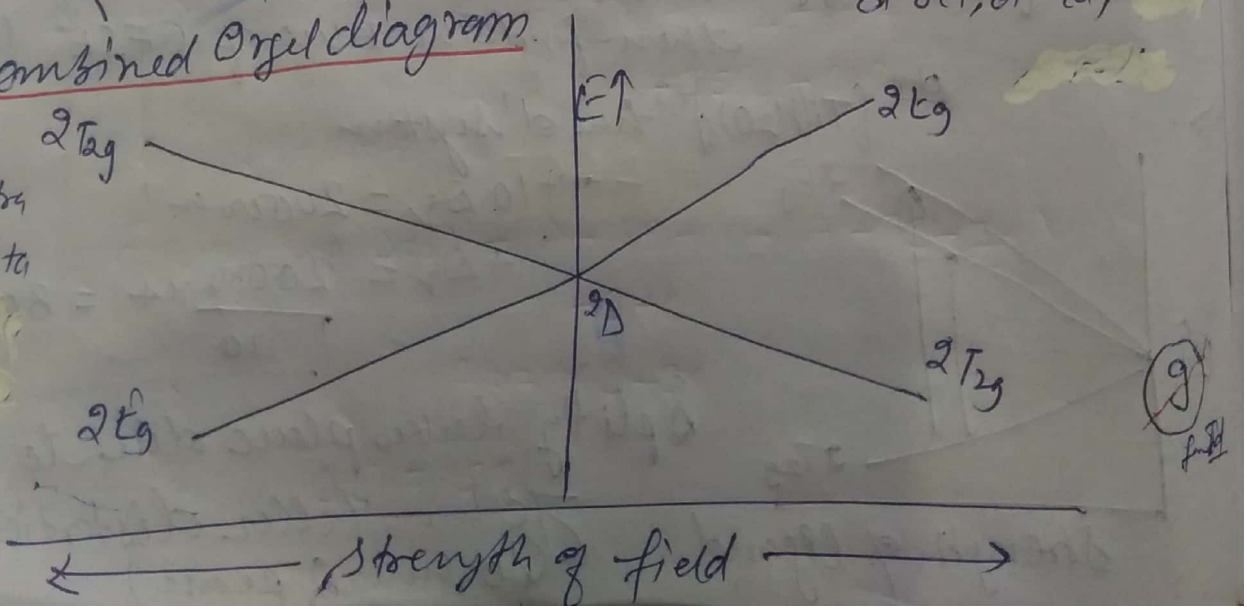






Combined Orgel diagram

d^1 oct, d^9 td,



d^1 tetra
d^9 octa

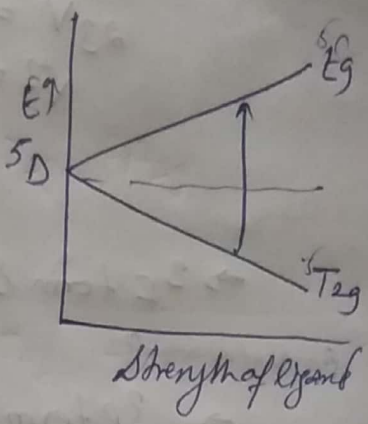
(9)

d^6 System (Oh) ⇒

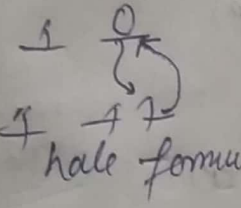
↑↓ | ↑ | ↑ | ↑ | ↑ S = 2, 2S+1 = 5, L = 2, G.S.T = ^5D

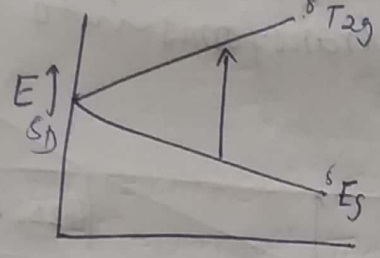
$[Fe(H_2O)_6]^{+2}$

$^5D \rightarrow {}^5T_{2g} + {}^5E_g$

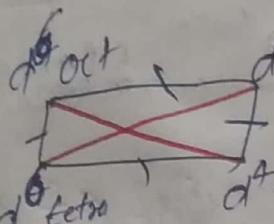


d^4 ↑ | ↑ | ↑ | ↑ | G.S.T = ^5D

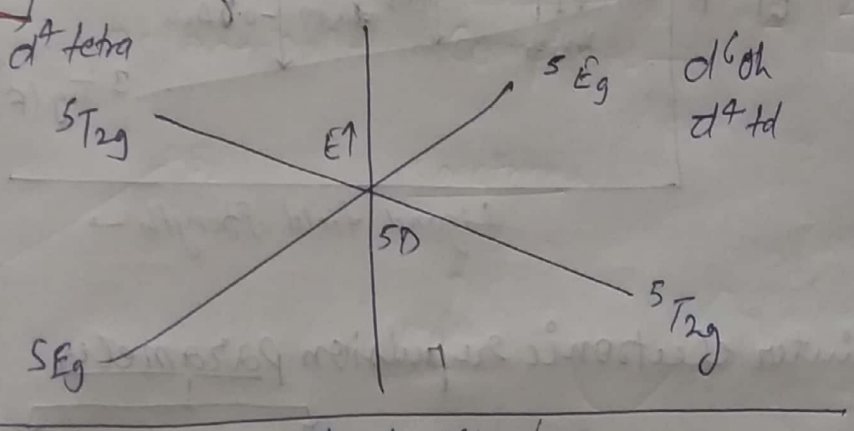




d^4 octa

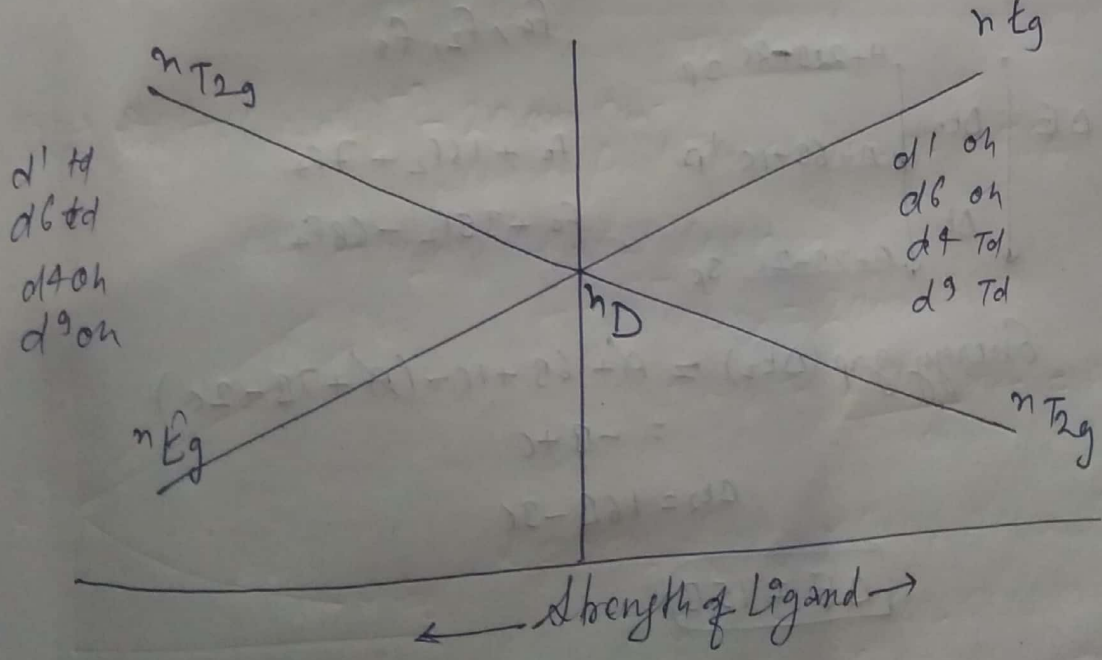


d^6 td
d^4 oh



d^6 oh
d^4 td

Combined Orgel diagram for d^1, d^4, d^6, d^9 ⇒ System



d^1 td
d^6 td
d^4 oh
d^9 oh

d^1 oh
d^6 oh
d^4 Td
d^9 Td

(9) Td