

Coordination Compounds

Ligand:
donating atom

An ion or molecule capable of a pair of electrons to the central via a donor atom.



Unidentate ligands

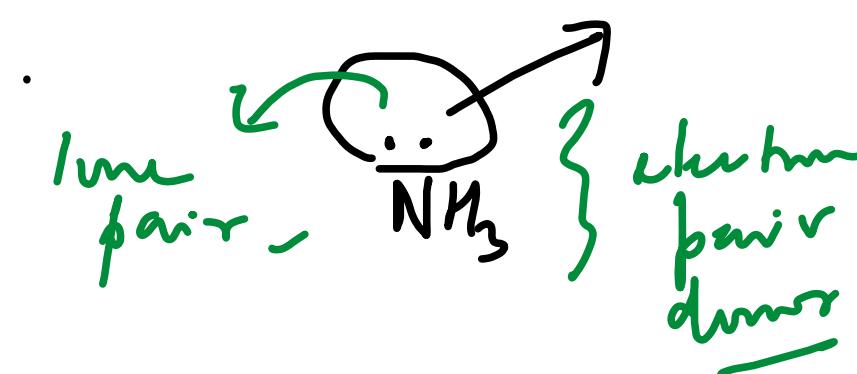
Ligand

↓

Bidentate Ligands

↓

Tridentate Ligands



Hexadentate ligands.

1. Unidentate ligands :- Ligands with only one donor atom. e.g. NH_3 , Cl^- , F^- etc.

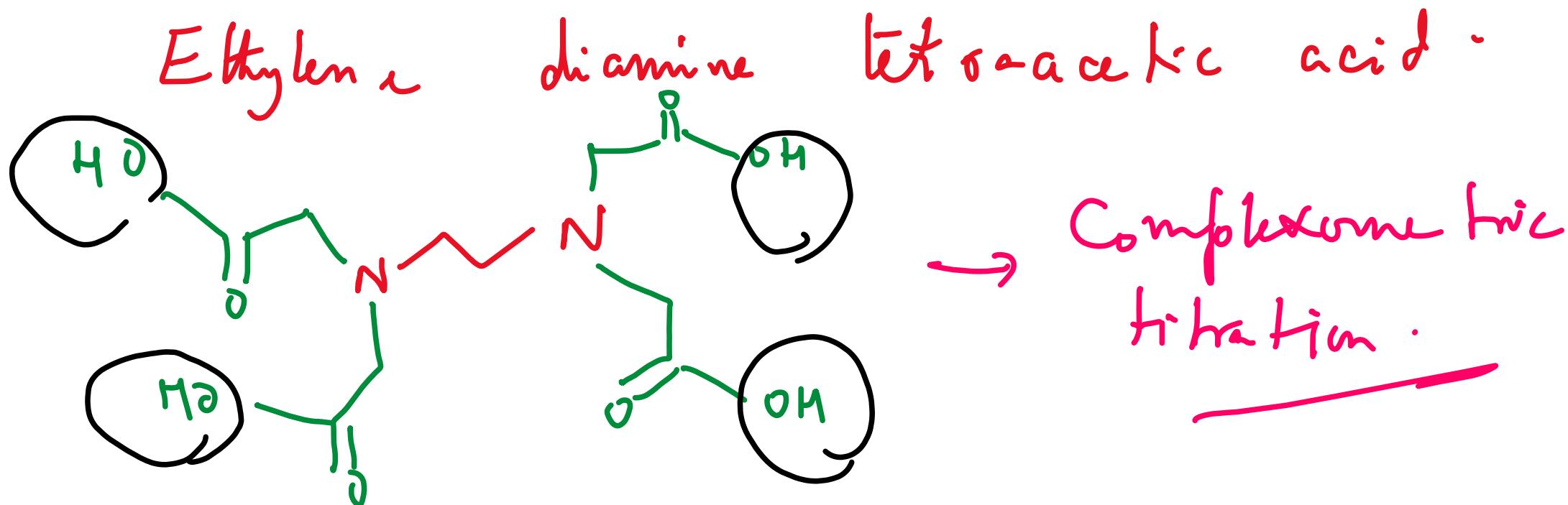
COON
|
 COO^-
2. Bidentate ligands: Ligands with two binding sites.

oxalic acid
 $\text{HOOC}-\text{COO}^-$

e.g. ethylene diamine, $\text{H}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{NH}_2$ → 2 binding sites
3. Tridentate ligands: Ligands with 3 donor atoms per ligand. e.g. Diethyl triamine.

4. Hexadentate ligand: Ligands which have six donor atoms per ligand. e.g - EDTA.

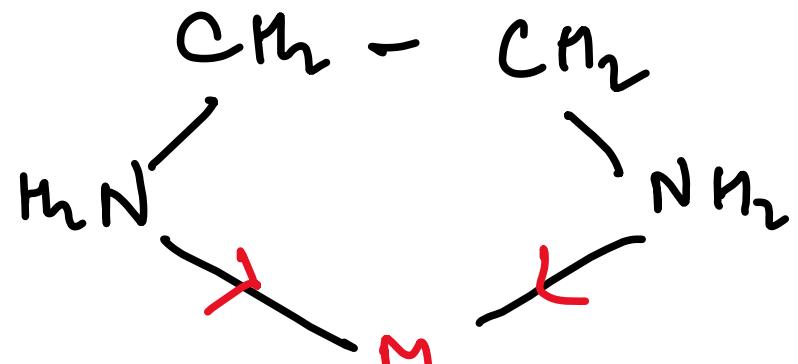
E-D-T-A



Chelating Ligands :-

Multidentate ligand

simultaneously coordinating to a metal ion through more than one i.e. multiple sites is called chelating ligand.



Chelation increases the stability of complex.

These ligands form a ring like structure called chelate.

Werner's Theory . 1893 .

First attempt to explain bonding in coordination compounds.

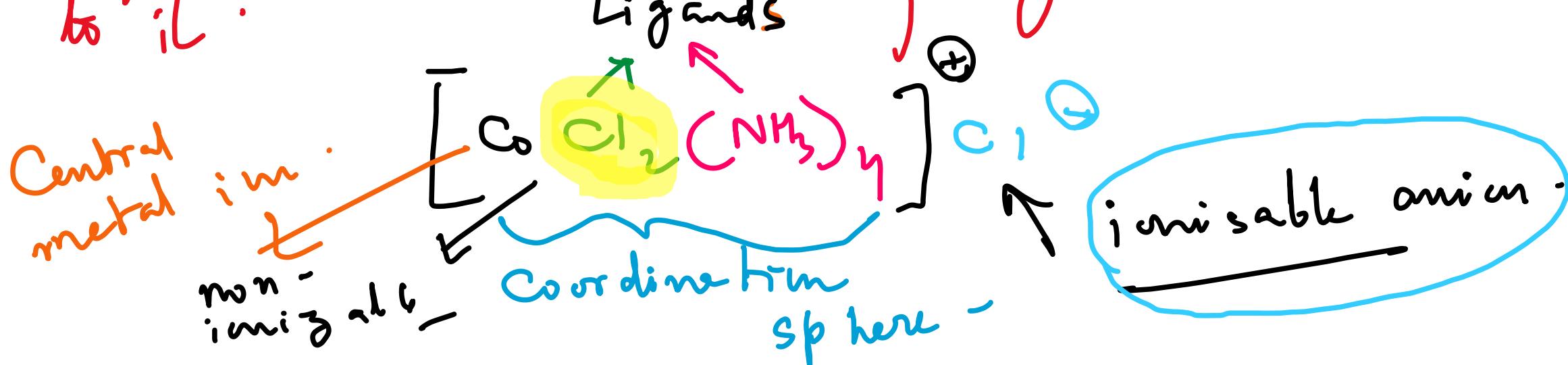
Alfred Werner - Nobel Prize in Chemistry in 1913

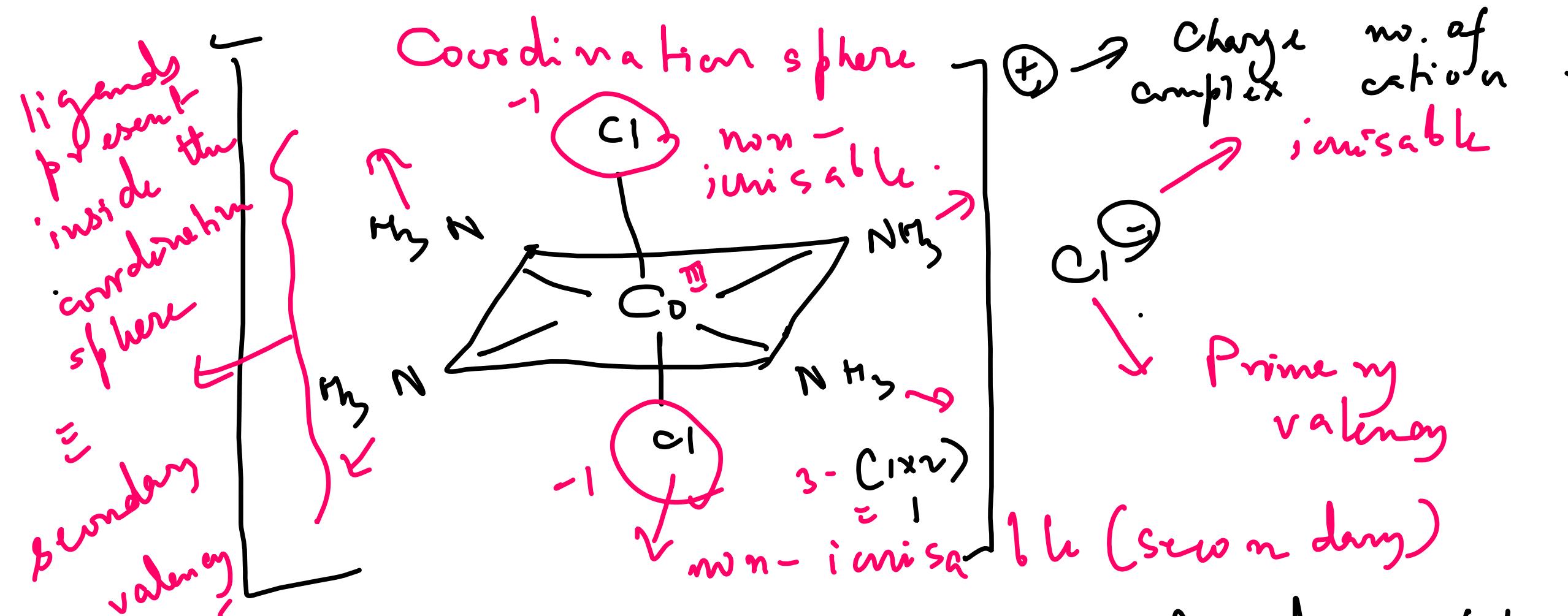
Werner's Theory:

1. Metals possess two types of valencies:
 - a) Primary valency
(ionizable)
 - b) Secondary valency.
(non-ionizable)

Primary valencies are satisfied by negative ions, while secondary valencies may be satisfied by neutral, negative or positive ions.

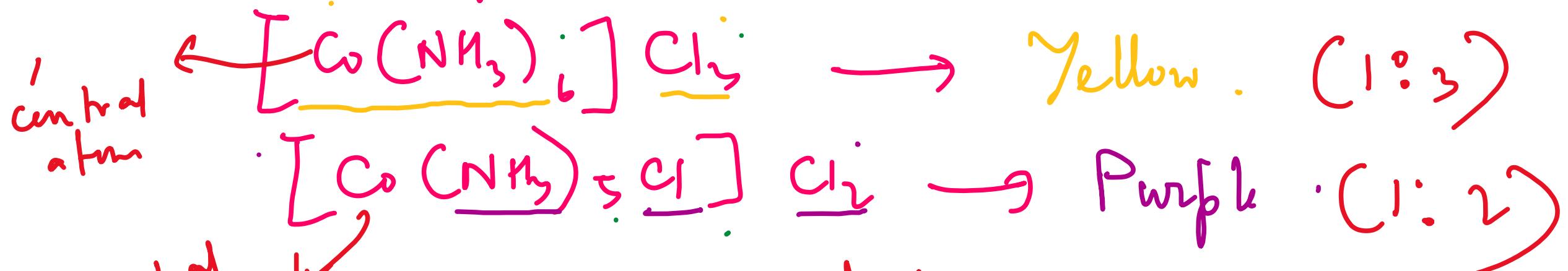
Secondary valency of a metal is equal to the number of ligands attached to it.





Secondary valencies have a fixed orientation in the coordination sphere -
 in the coordination sphere ~ $[Co^{III}(NH_3)_5Cl]Cl_3$
 Primary valency = 3 Cl
 Secondary valency = 5 NH₃

Werner's studies on Co^{3+} complexes allowed him to propose a structural model for metal complexes with c. n. - c.



Werner found that $[\text{Co}(\text{NH}_3)_6] \text{Cl}_3$ and $[\text{Co}(\text{NH}_3)_5 \text{Cl}] \text{Cl}_2$ were 1:3 and 1:2 electrolytes.

Unexpectedly, two different compounds were known electrostatically.



1 : 1

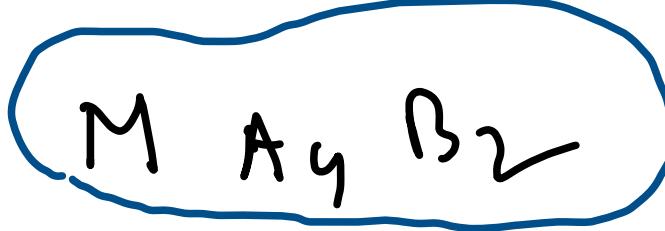
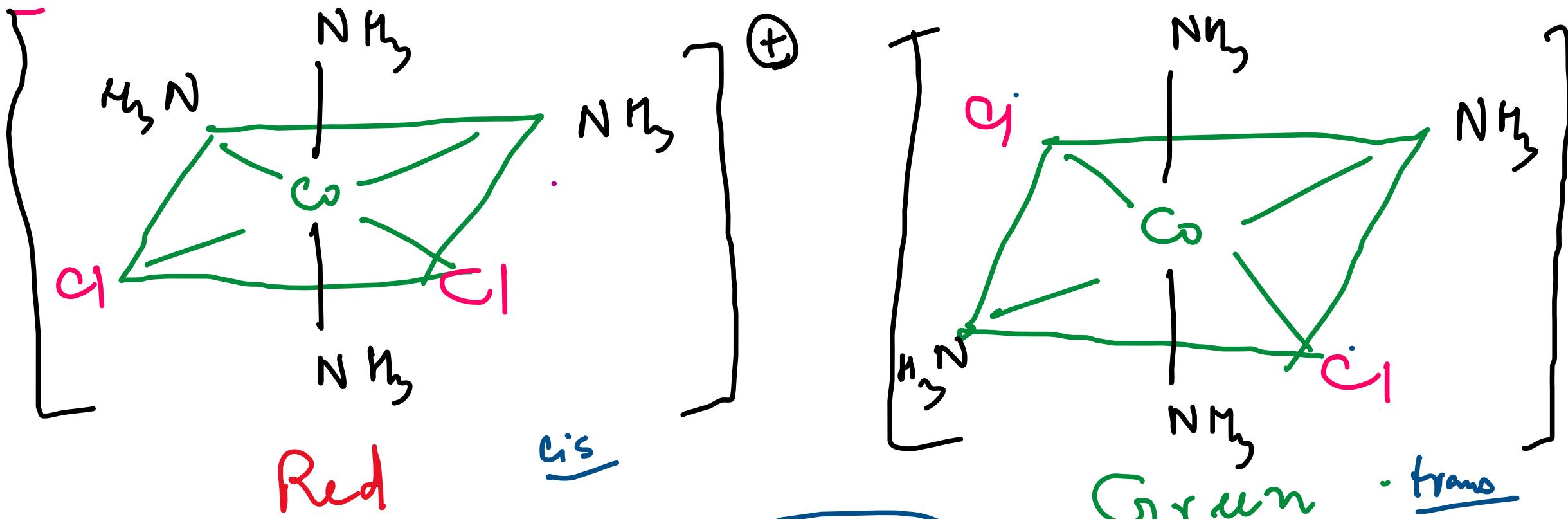
Red

Green

Because both compounds had the same chemical composition and the same no. of groups of the same kind of atom.

attached to the same metal, there must be something different about the arrangement of the ligands around the metal ion. Werner hypothesized the + six ligands had to be arranged in an octahedron at because that was its only structure, which was consistent with the existence of two, and only two arrangements of ligands.

$$[Co(NH_3)_6 Cl_2]Cl$$



In Werner's time, many complexes of $\text{M} \text{Ag} \text{B}_2$ were known but the general formula was not more

Two different compounds with the same composition had been prepared for any metals. To confirm Werner's reasoning, calculate the maximum number of different structures that are possible for six-coordinate $M(A_6B_2)$ complexes with each of the three most possible symmetrical structures:

a hexagon, a trigonal prism, octahedron. What does the fact that no more than two forms of any

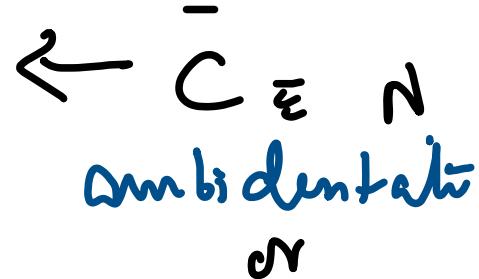
May Br complex were known till you
about the 3d structures of these complexes.

Given: three possible structures and
the no. of different forms of MA_3B_2 complexes.

Ambidentate Ligand: A ligand that may
have more than one kind of donor
sites but at a time only one kind of
donor site is utilized for donation.

①

Mono dentate & am bidentate



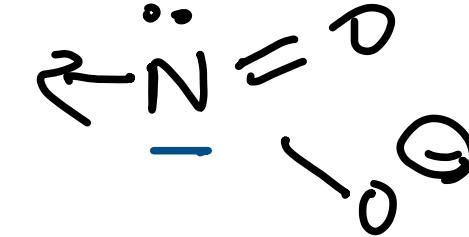
isocyanide



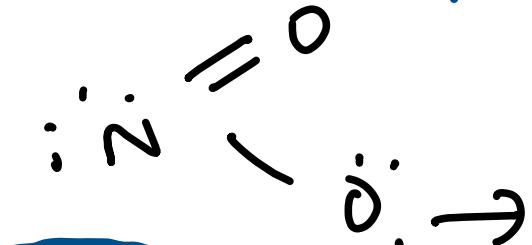
or



or



or



mono dent + anti
and
am bidentate

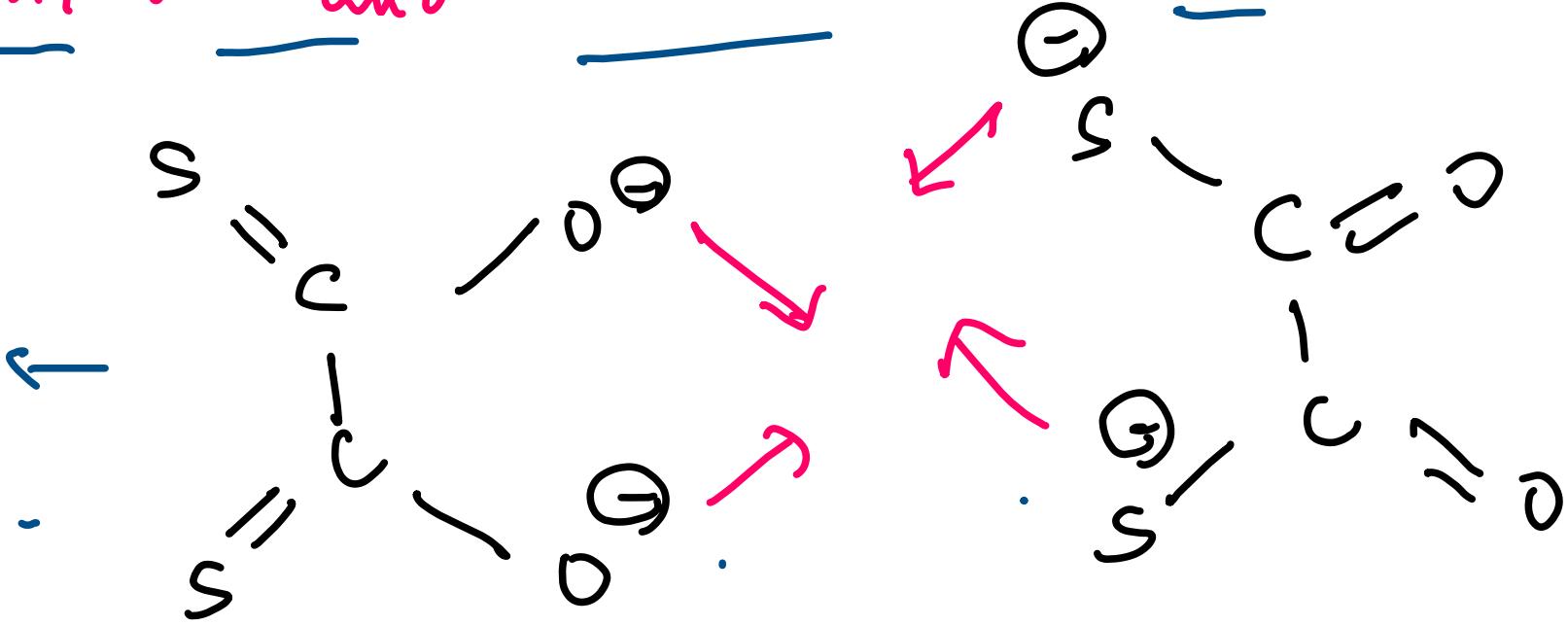


2

Bidentate and ambidentate

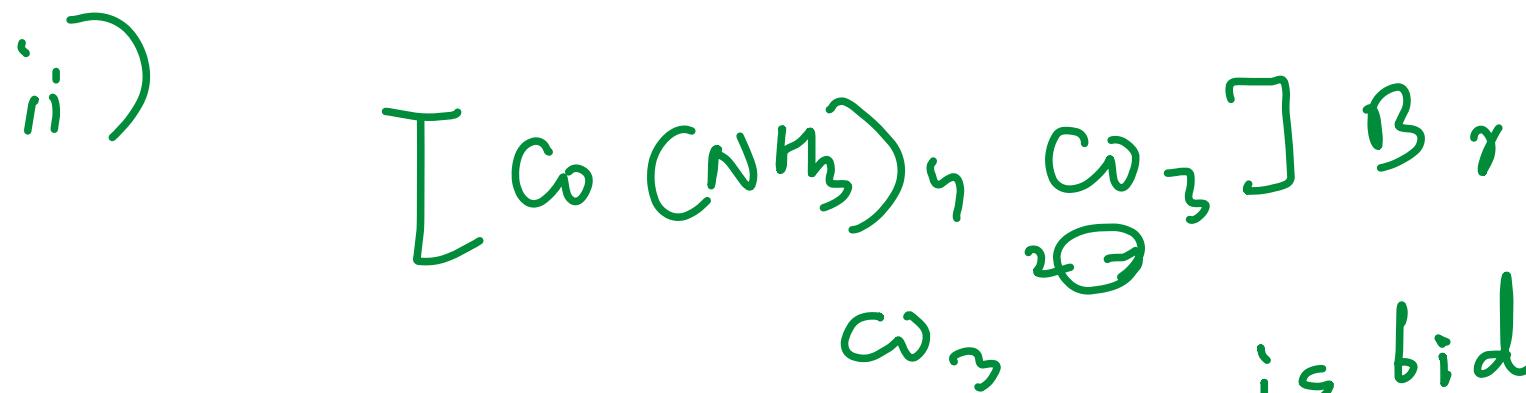
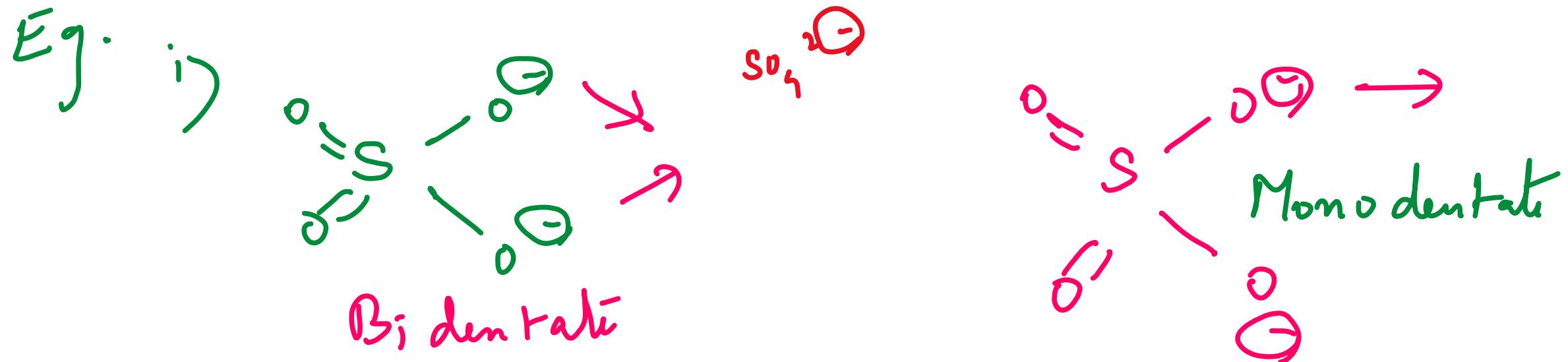
can bind
via both

sulfur &
oxygen



Diethoxalate

Flexidentate ligand: A ligand which shows variable dentativity.



Nomenclature of Coordination Compounds

Summary of rules of nomenclature as recommended
by I.U.P.A.C.

- i) The positive ion (cation) is named first followed by the negative ion (anion)
- ii) When writing the name of a complex, the ligands are quoted in alphabetical order, regardless of their charge (followed by metal)
- iii) For the complex entity, the metal is

is named first, then the coordinate group are listed in the order of negative ligands, neutral ligands, positive ligands (and alphabetically according to the first symbol within each group).

The name of -ve ligands end in O.

F - fluor, O₂ - ox, N₂ - nitro - etc.

Neutral group have no specific endings.

Positive groups end in - ' - ium '
e.g., NH₂ - NH₂ → hydrazinium -

iv) The number of ligands is indicated by adding prefixes of di, tri, tetra, penta etc. for 2 , 3 , 4 , 5 etc. entities of the ligand.

Exception: When the name of the ligand includes a number e.g. ethylene diamine

$[\text{Co}(\text{NH}_3)_6] \text{Cl}_3$

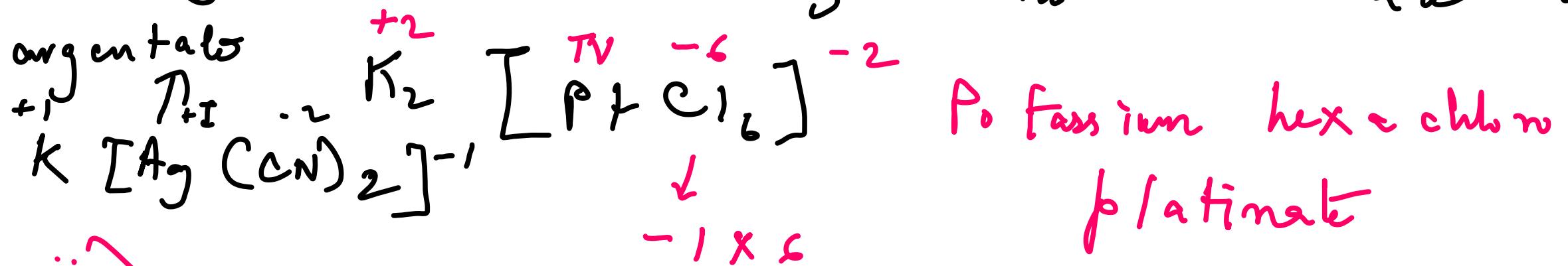
Hexamine cobalt(II) chloride -

roman numeral in bracket with bracket

v) The oxidation no. of the central metal is shown by a roman numeral in brackets immediately

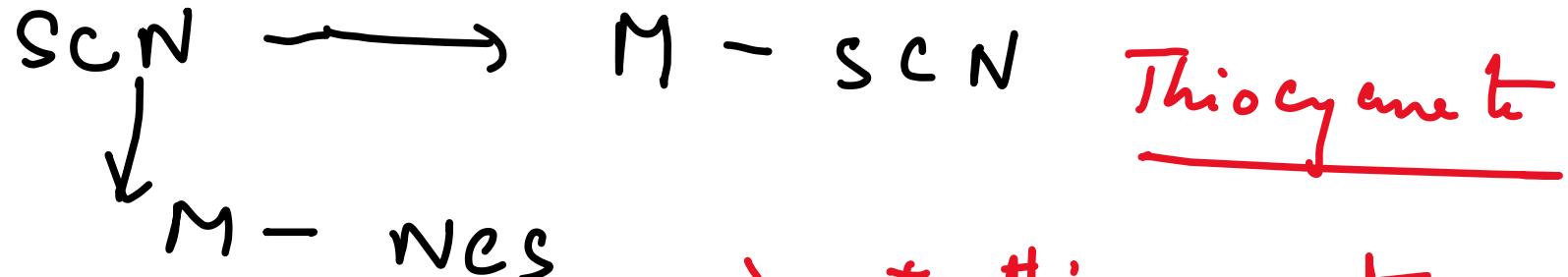
after the name of the metal.

vi) Complex positive ions and neutral molecules have no specific ending, but complex negative ions always end in -ate.



vii) Sometimes, a ligand may be attached through different atoms. Thus $\text{M}-\text{NO}_2$, nitro and $\text{M}-\text{ONO}$ is called.

nitrile.



Sys I automatically, like e

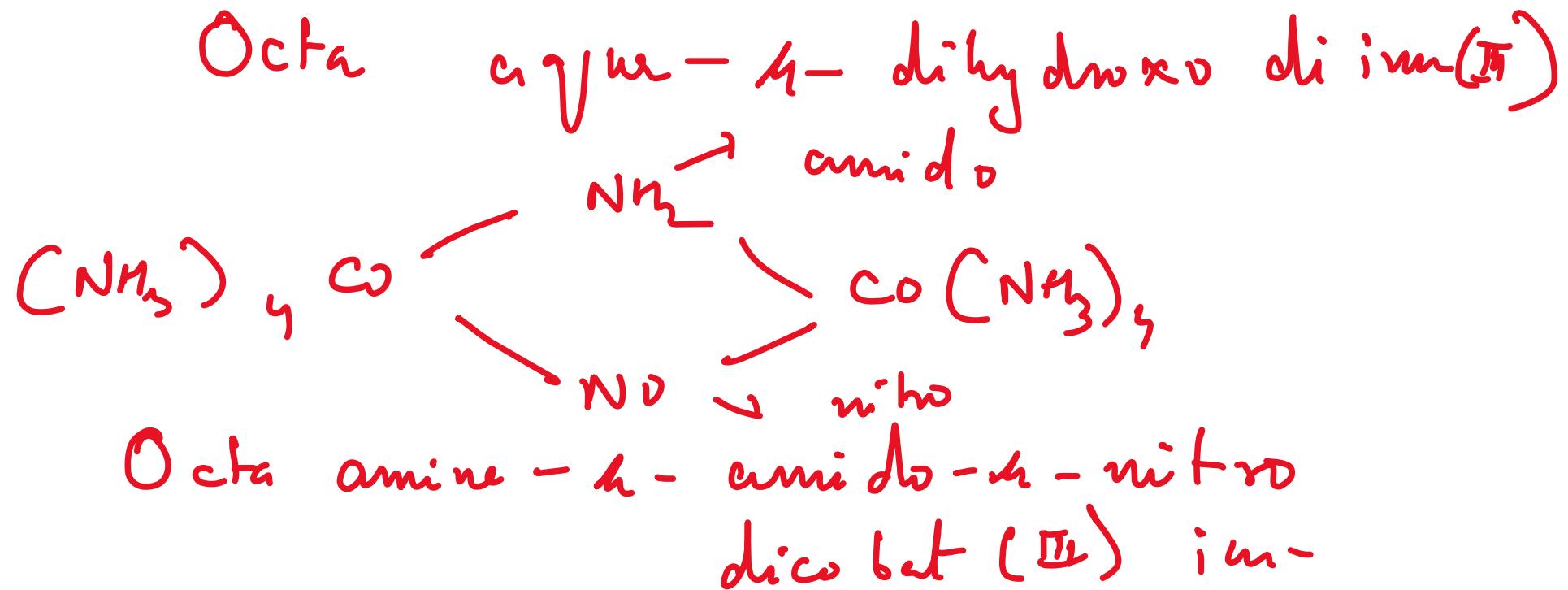
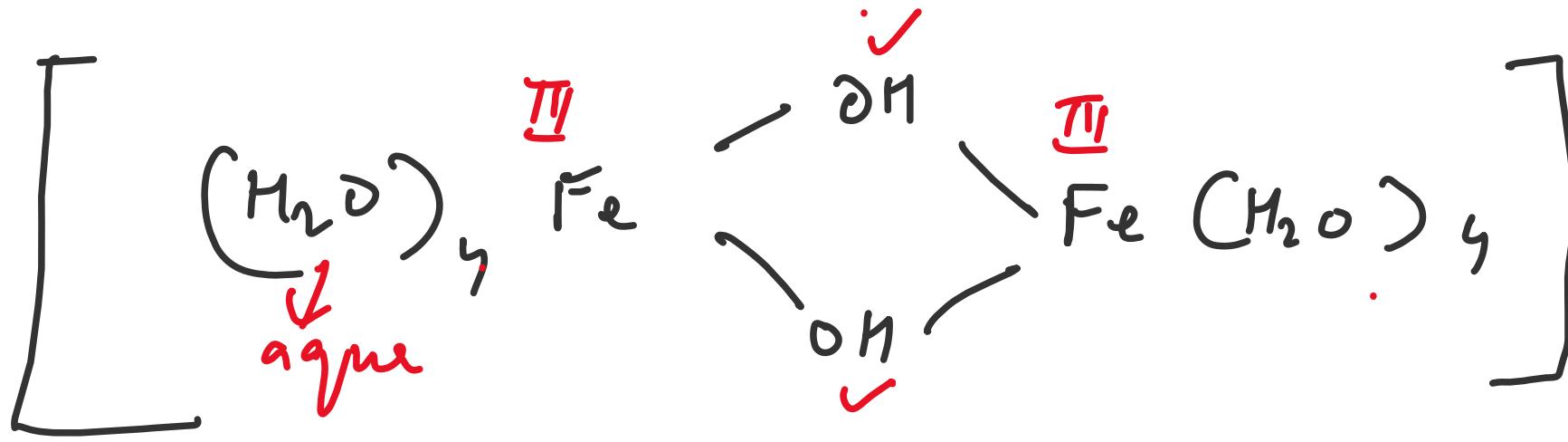
may be name as this cyanato-S or this cyanato-N

Specify the + binding site

This indicates how the atom which atom
is bound to the metal.

⑧

If the complex contains two or more metal atoms, it is termed polymeric. The bridging groups which link the two metal atoms together are indicated by the prefix a or more bridging If there are two same kind, this is indicated by di-, tri-, etc. Bridging groups are listed alphabetically with the other groups unless the symmetry of the molecule allows a simpler name.



Cations :

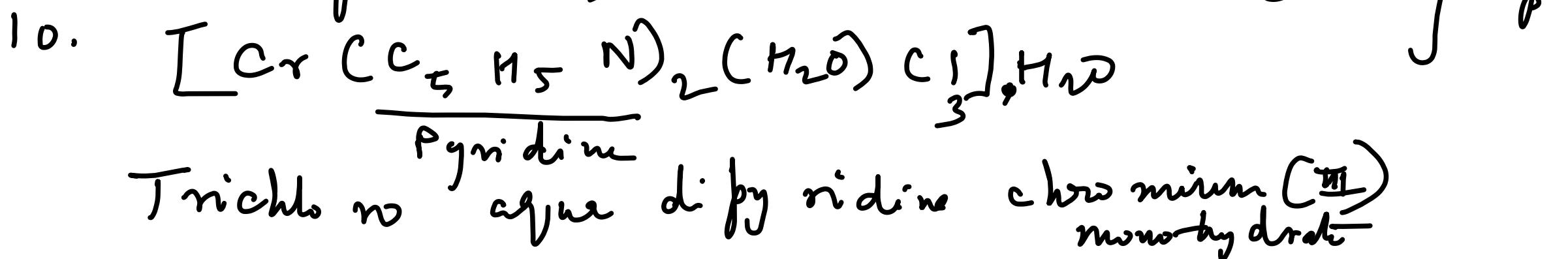
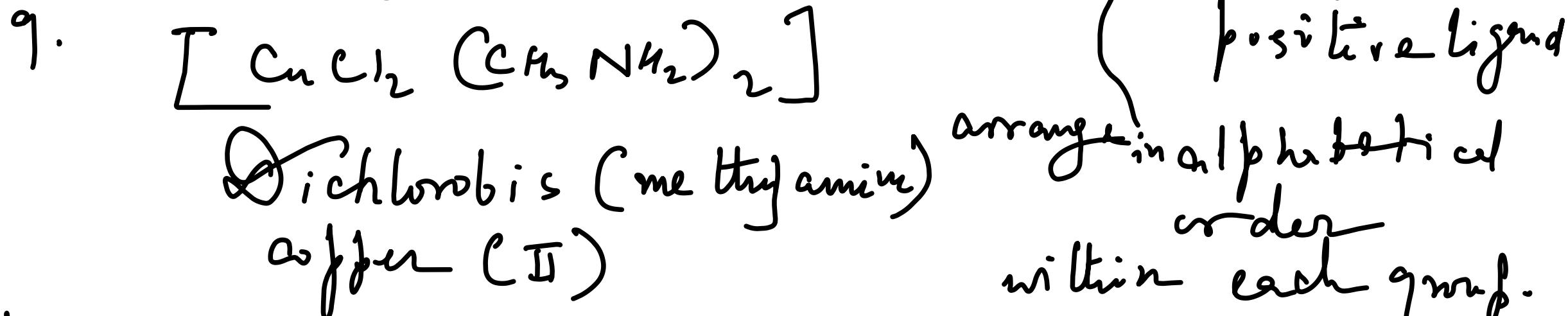
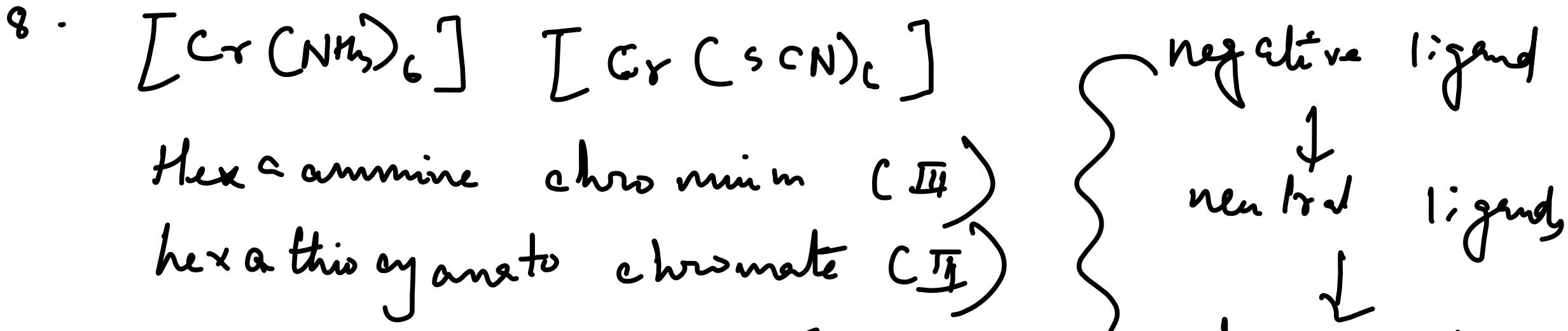
1. $[\text{Ag}(\text{NH}_3)_2]^{\text{Cl}} \rightarrow$ Di ammine Silver(I) chloride -
2. $[\overset{\text{III}}{\text{Cr}}(\text{H}_2\text{O})_4\text{Cl}_2]^{\oplus} \rightarrow$ Diclow. tetra- aqua chro minum (III) cation -
3. $[\overset{\text{II}}{\text{Fe}}(\text{H}_2\text{O})_6]^{50\%} \rightarrow$ Hexa - aquo iron (II) sulphate

Anions :

1. $\overset{+4}{\text{K}}, \overset{\text{II}}{[\text{Fe}(\text{CN})_6]}^{\text{-6}} \rightarrow$ Pot. hexa cyano ferret (II)
2. $\overset{+3}{\text{Na}}, [\text{Co}(\text{NO}_2)_6] \rightarrow$ Sod. hexa nitro cobaltate (VII)

More examples -

1. $[\text{Co}(\text{NH}_3)_5\text{Cl}]^{2+}$: Chloropentaammine cobalt(II) cation.
2. $[\text{Co}(\text{NH}_3)_4\text{Cl}_2]^+$: Dichlorotetraammine cobalt(III) ion.
3. $[\text{Co}(\text{NH}_3)_6]\text{Cl}_3$: Hexaammine cobalt(IV)
4. $[\text{Pb}(\text{OH})_4]^{2-}$: Tetrahydroxydianino plumbate(II) chloride.
5. $[\text{Ag}(\text{NH}_3)_2]\text{Cl}$: Diammine silver(I) chloride.
6. $[\text{Cr}(\text{en})_3]\text{Cl}_3$: Tris(ethylene diamine) chloro chromium(III) chloride.
7. $[\text{Co}(\text{NH}_3)_5\text{H}_2\text{O}]\text{Cl}_3$: Pentaaammine aqua cobalt(IV) chloride.

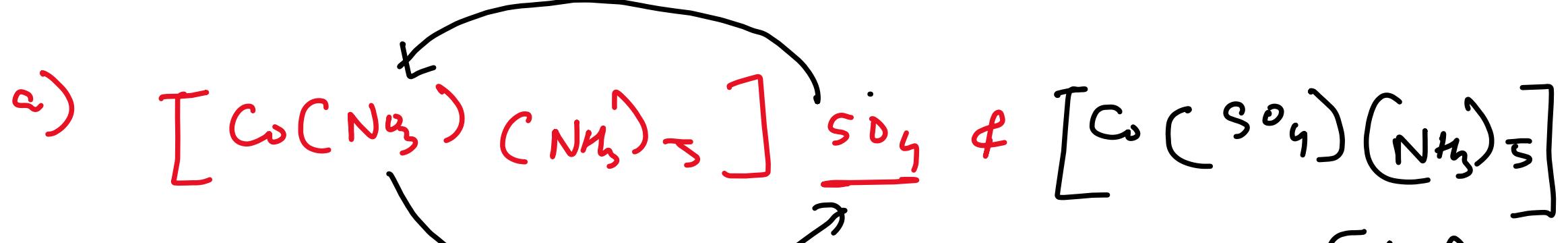


Isomerism

Compounds with same chemical formula but different structural arrangements are called isomers and the phenomenon is called isomerism.

Types of Isomerism in Coordination Compounds

- i) Ionisation isomerism - This type of occurs when the counter ion in a coordinate ion compound is itself a potential ligand.



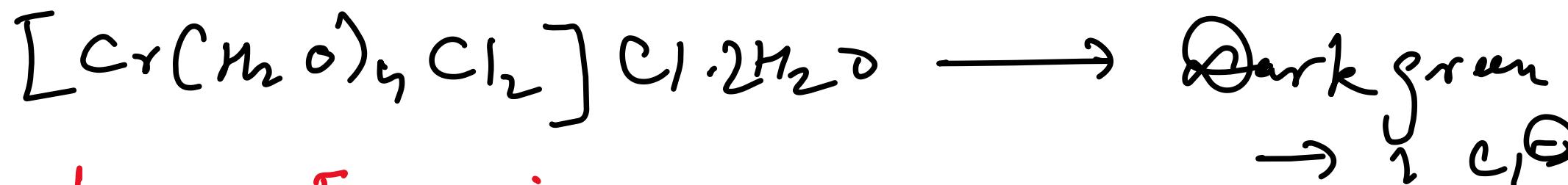
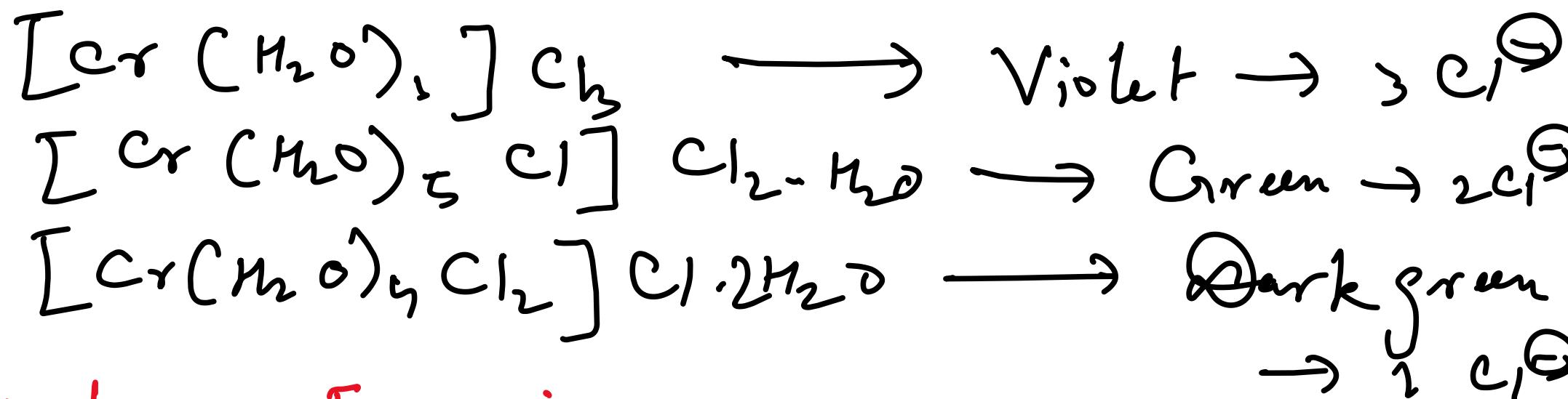
$\left\{ \begin{array}{c} \text{Br}^- \\ \downarrow \\ \text{in in} \\ \text{s, h} \end{array} \right.$ $\left\{ \begin{array}{c} \text{Cl}^- \\ \downarrow \\ \text{in in} \\ \text{s, h} \end{array} \right.$

imagine differently,

ii) Hydrati Isomerism:



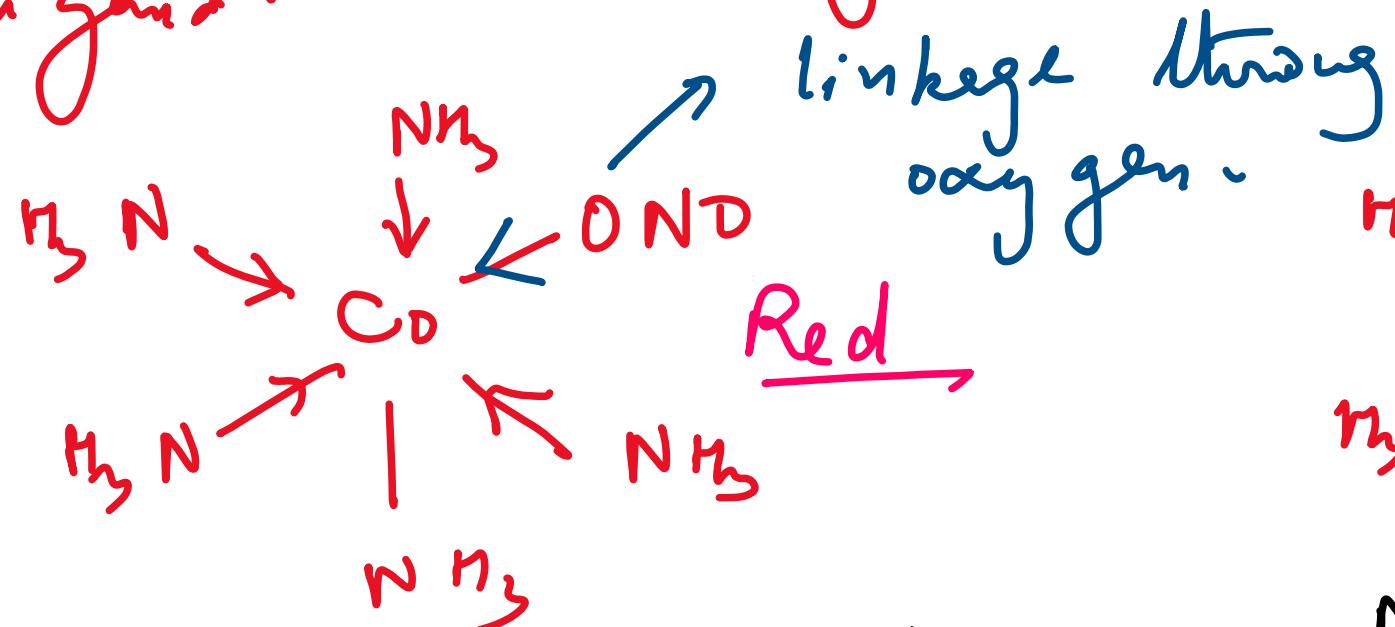
Conductivity measurements and quantitative preparation show that 3 isomers of $\text{CrCl}_3 \cdot \text{H}_2\text{O}$ exist.



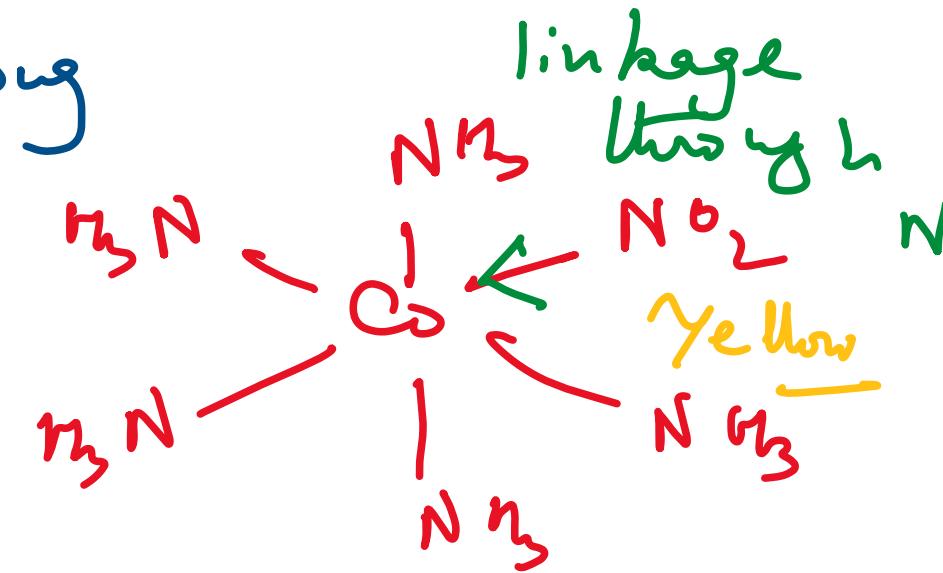
Linkage Isomerisms

Isomers involving ambidentate ligands.

Linkage isomerism is the existence of coordination compounds that have the same composition differing with the connectivity of the metal to the ligand.



Nitro pentammine cobalt(III)



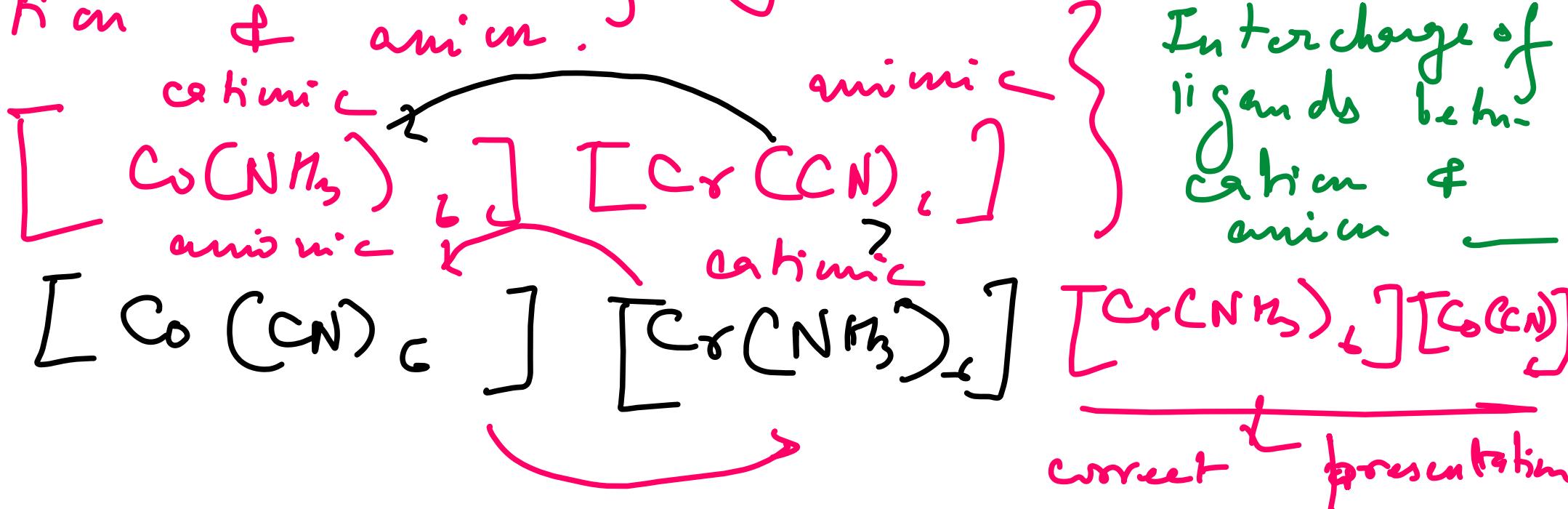
Nitro pentammine cobalt(IV) i.e.

i.)

Coordination Isomerism: When both

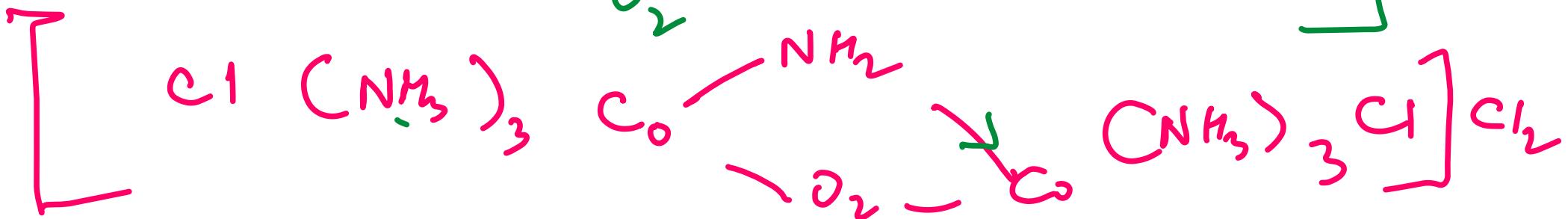
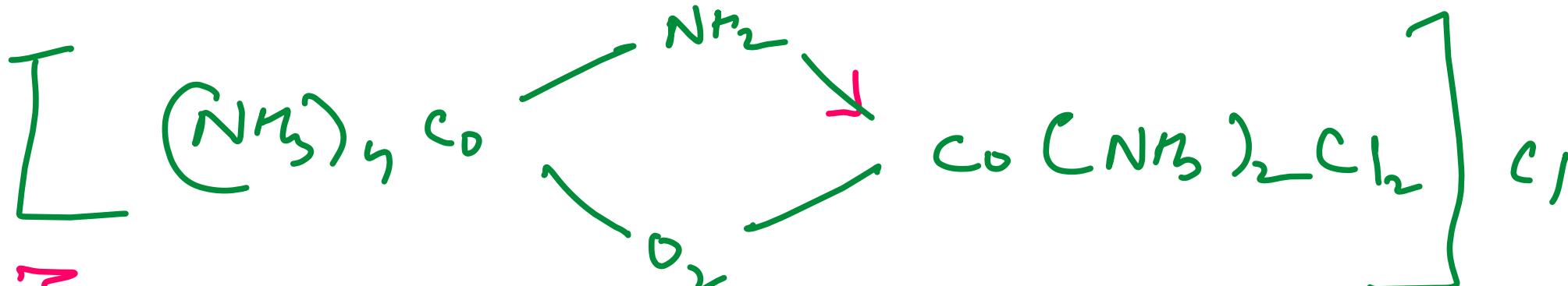
the positive and negative ions are complex ions, isomerism may be caused by inter change of lig and between the

cation & anion.



v) Coordination Position Isomerism.

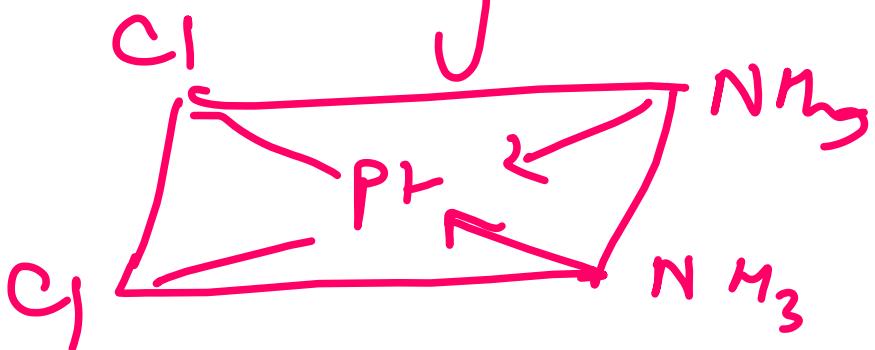
In poly nuclear complexes, exchange of ligands between the different metal nuclei gives rise to positional isomerism.



Geometric

Isomerism

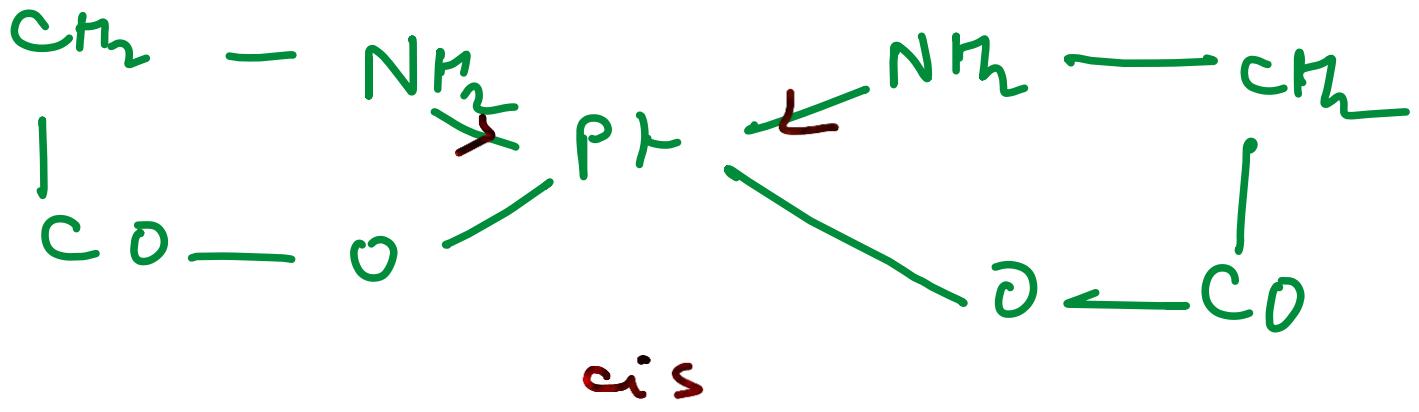
In disubstituted complexes, the substituted groups may be adjacent or opposite to each other. They give rise to geometric isomerism.



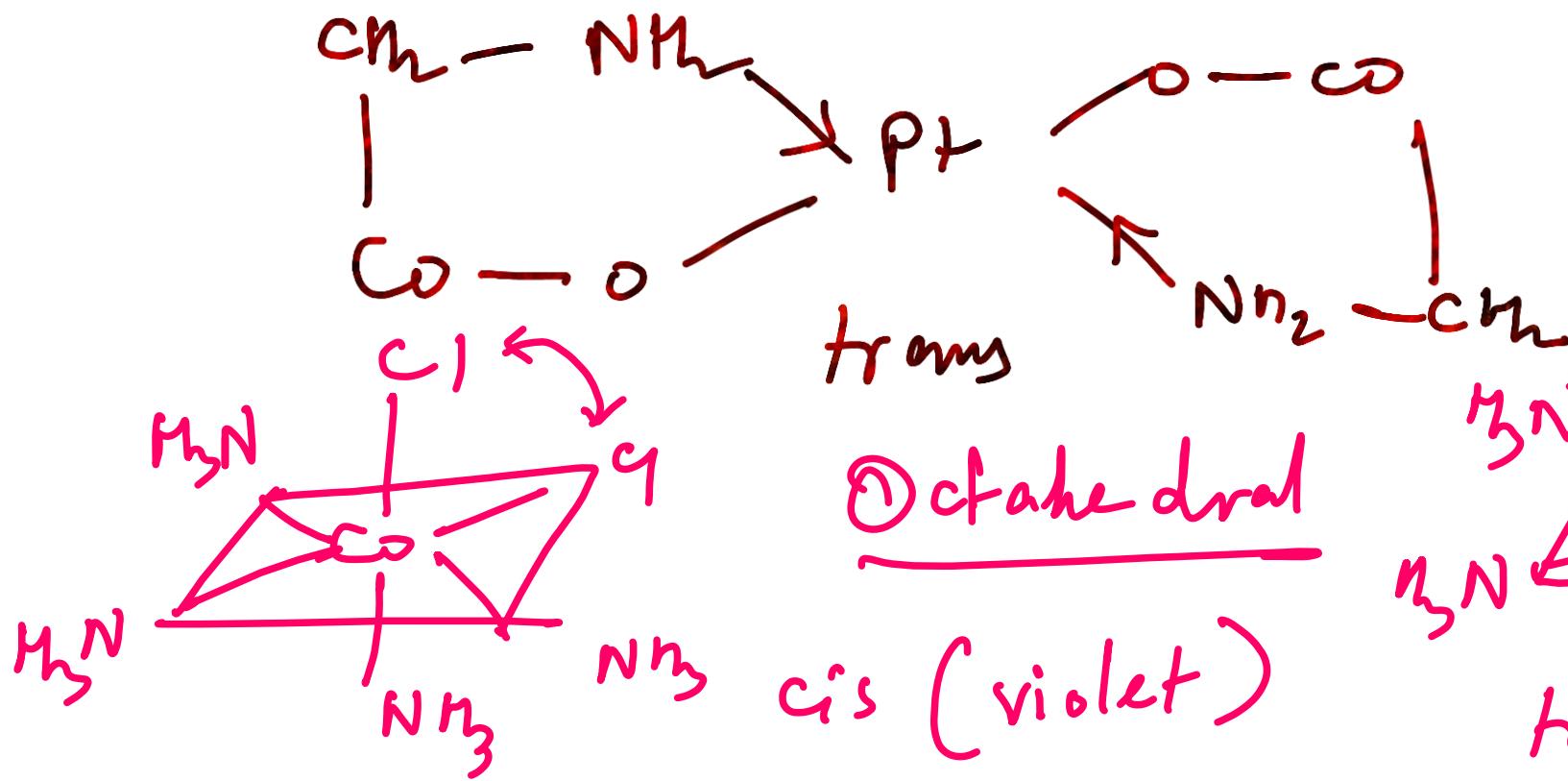
cis



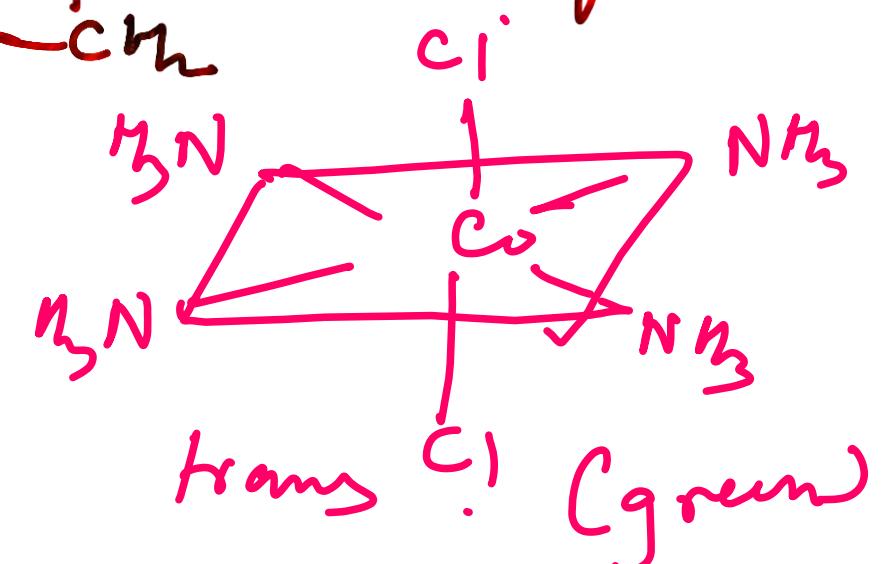
MA_2B_2



Square Planar



Cis and
Trans by cis
complex.



Square Planar :- Coordinate fission w.r.t.



anti cancer agent

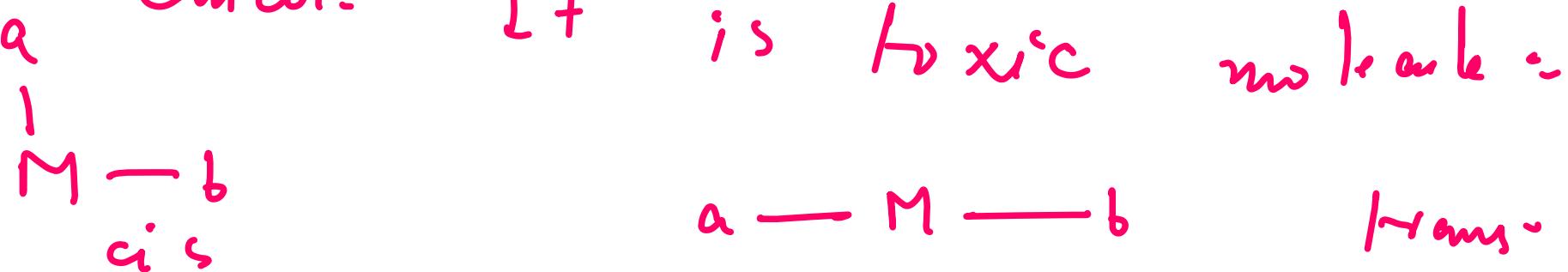
trans - Pt Cl₂(NH₃)₂ is inactive

against

cancer

If

is toxic molecule :-



Octahedral :

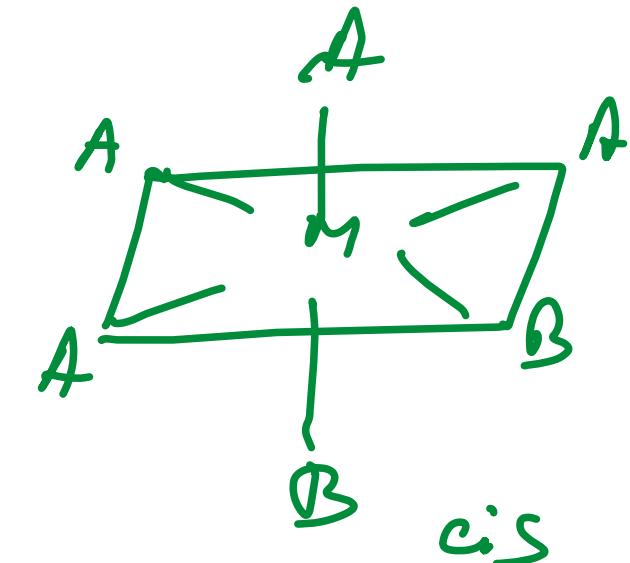
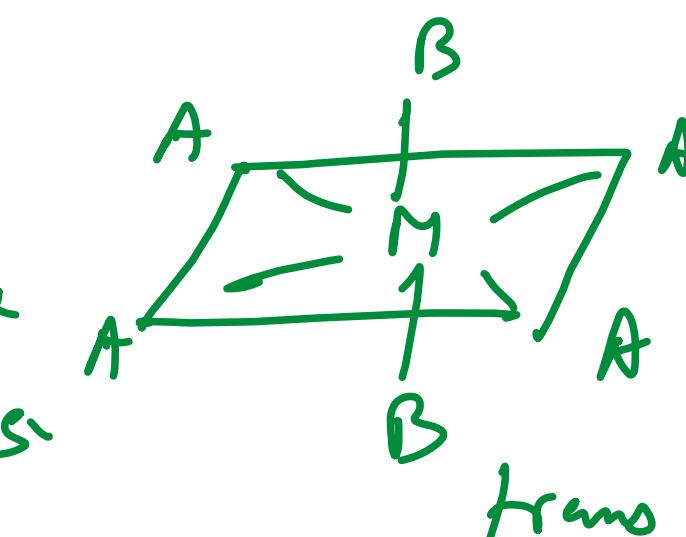


2 isomers possible
cis - & trans



Optical isomerism

Coordination no : 6



(face - and mer -)

(2 * cis - and 1 - trans)

Octahedral complex.

Coordination Chemistry

Werner also attempted to find the shape of the complexes.

The possible arrangements of six groups around one atom are -

- i) planar hexagon or ii) trigonal prism .
- iii) octahedron .

Werner compared the number of isomeric forms he had obtained with the artificial ones for each of the possible shapes

Number of isomers predicted and actually found.

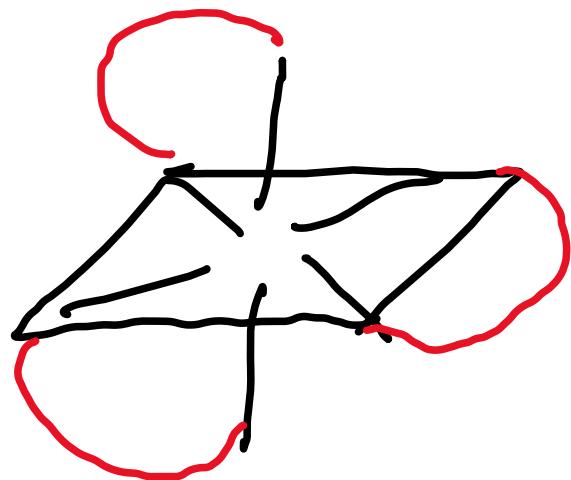
Complex	Observed	Predicted	Octahedral	Planar hexagon	Trigonal Prism
MX_6	1	.	1	1	1
MX_5Y	1	.	1	1	1
MX_4Y_2	2	.	2	3	3
MX_3Y_3	2	.	2	3	3

These results strongly suggest that these complexes have an octahedral shape.

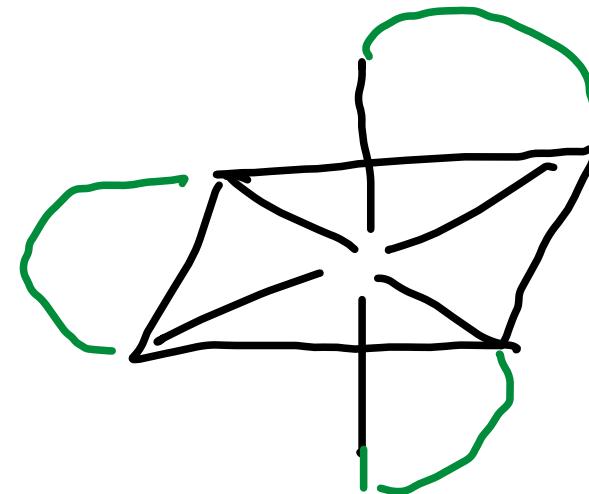
This was not absolute proof,
as it was just possible that the correct
condition were not for preparing all the isomers
found. More recently, X
ray structures have been determined and
these establish that the shape is octahedral.

More recently, with a bidentate ligand
such as ethylene diamine ($1,2$ -diaminopropane)
two optically active isomers of octahedral

com plex have been found.



mirror



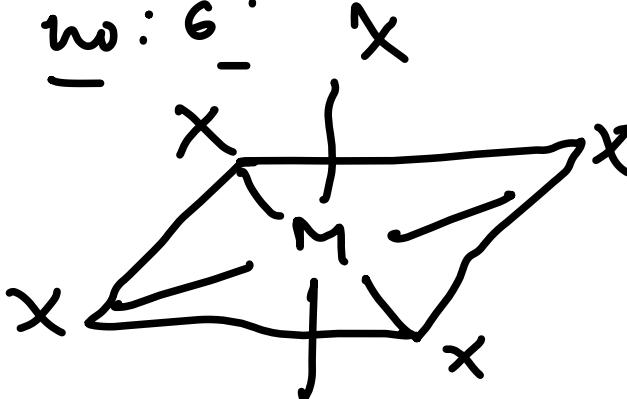
Optical
isomers in
in coordination
complex

Octahedral complex \rightarrow Possible combinations



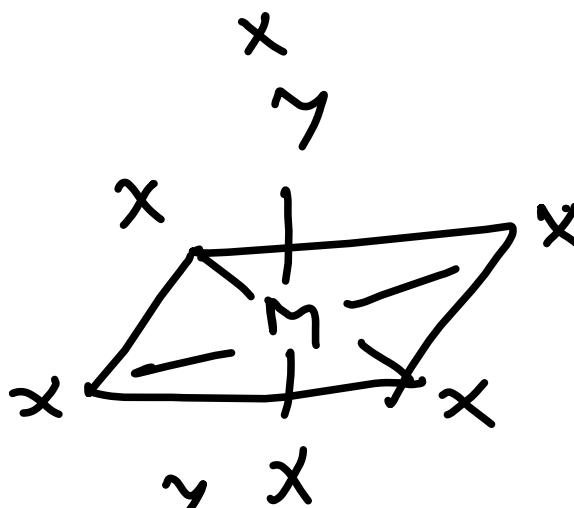
Coordination no: 6

MX_6

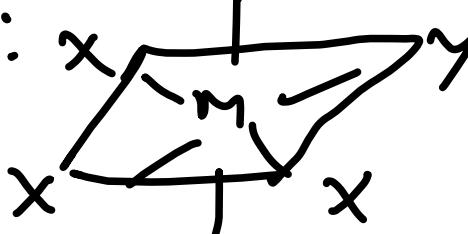


Only one form

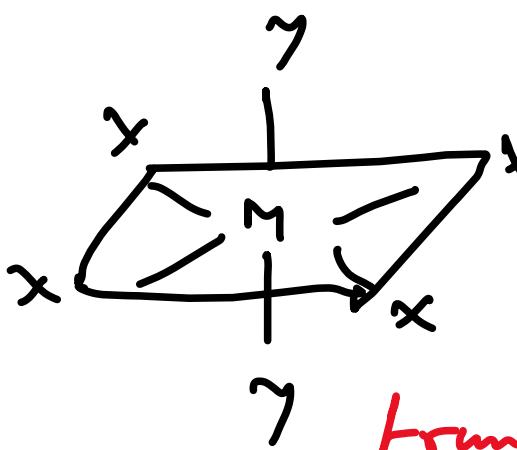
MX_5



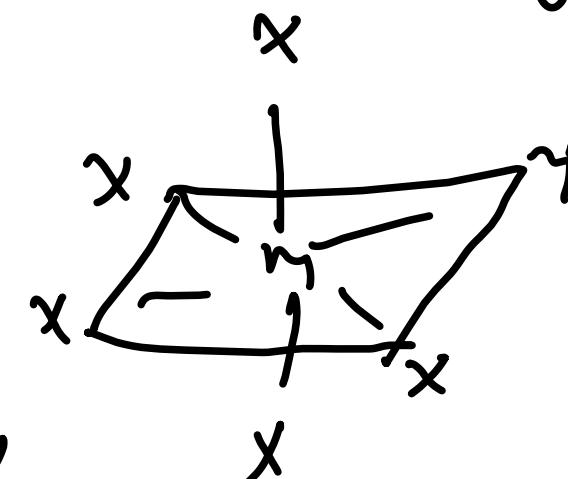
$MX_4 Y_2$



cis



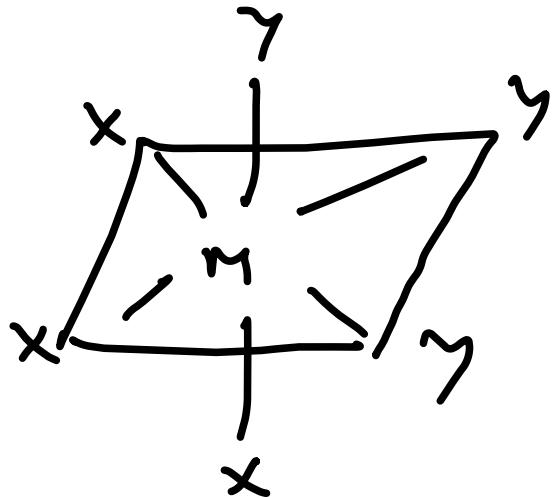
trans



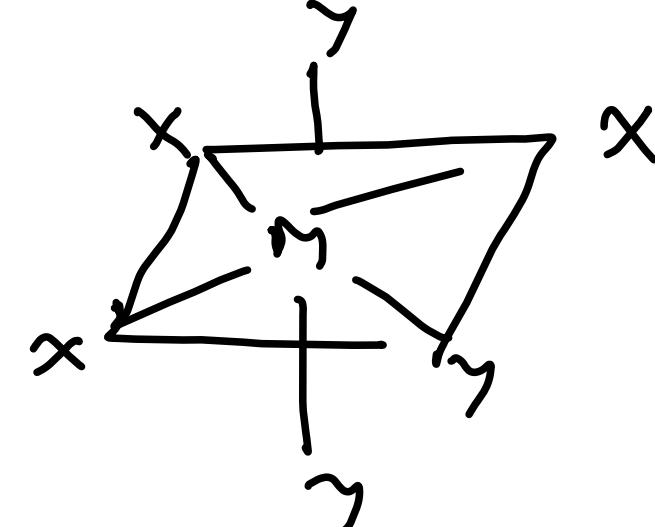
Only one form as
all six corners
vertices
are equivalent.

Two isomers are possible

$MX_3 Y_3$



facial (Fac-)



Meridional. (Mer-)

Two isomers are possible: facial & meridional

Isomerism in - correlative form no : 4.

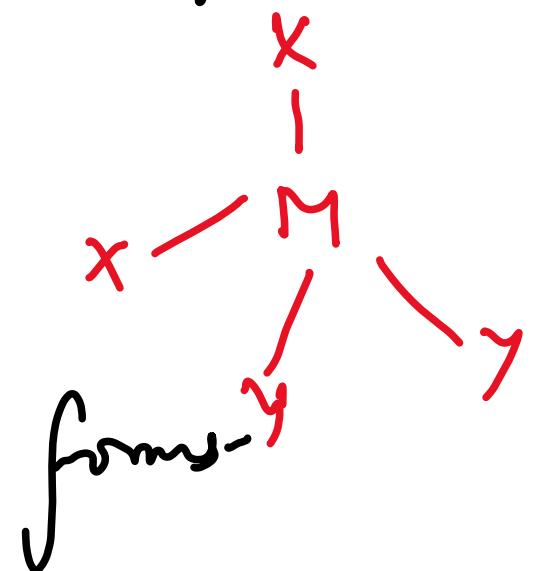
Just like octahedral complex, Werner studied a range of complexes such as $[Pt^{\text{II}}(C_6H_5)_2Cl_2]$ C.N. = 4

and $\left[\text{Pd}^{\text{II}}(\text{NH}_3)_2\text{Cl}_2 \right]$. Because the c-n.
is 4, two shapes are possible:

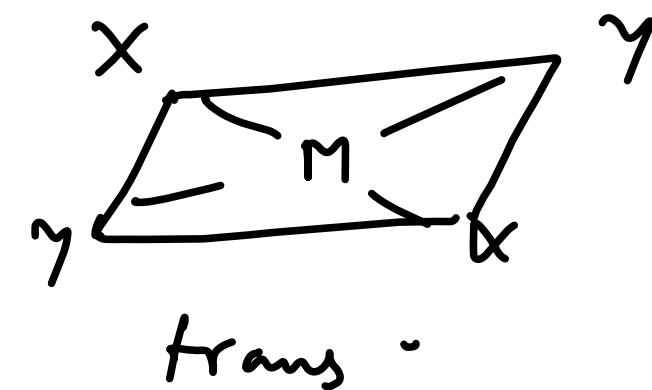
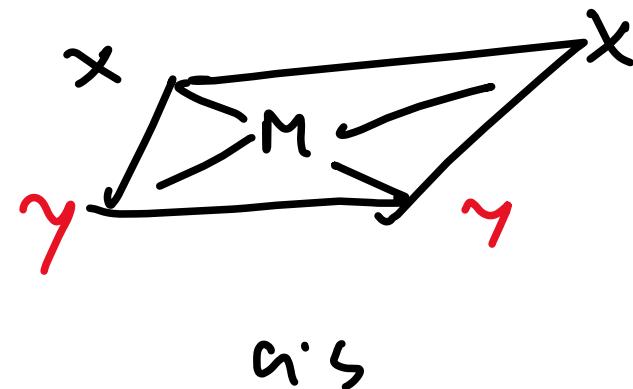
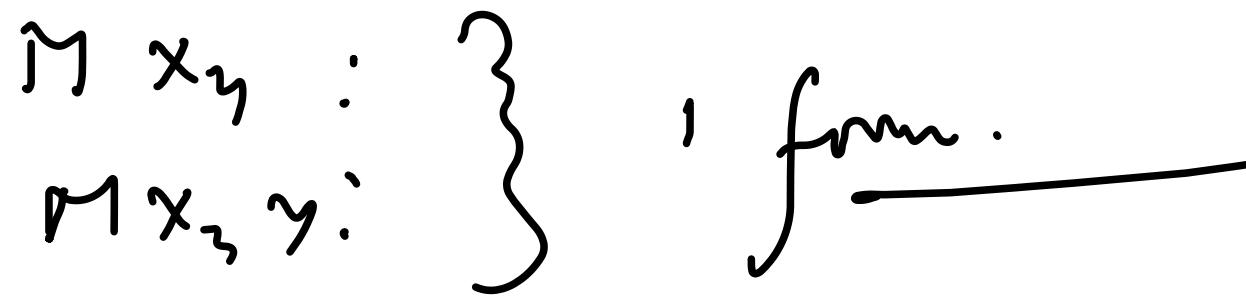
- i) Tetrahedral and ii) Square planar.

Werner was able to prepare two different isomers for these complexes.

A tetrahedral complex can exist in only 1 form but a square planar complex can exist in two isomeric forms -



This proved that these complexes are square planar rather than tetrahedral.



Effective atomic number (EAN)

Physically, EAN signifies the number of electrons available around a central atom within a complex including the electrons accepted from ligands. It is thermometrically defined as —

E.A.N. of a central atom in a complex =
Atomic no. of the central atom (Z) -
Coxide ion no. of the central atom with sign
+ (number of electrons from the ligands..)

Coordination Chemistry

1. Valence bond Theory : (VBT)
2. Crystal field Theory. (CFT)
3. Molecular Orbital Theory (MOT)

1. V.B.T :

This theory was developed by Pauling -

Coordination compounds contain complex ions in which ligands form coordinate

bond to the metal. Thus, the ligand must have a lone pair of electrons, and the metal must have an empty orbital of suitable energy available for bonding.

The theory considers which atomic orbitals on the metal are used for bonding. From this, the shape and stability of the complex are deduced -

Limitation: i) Most transition metal complexes are coloured, but the theory provides

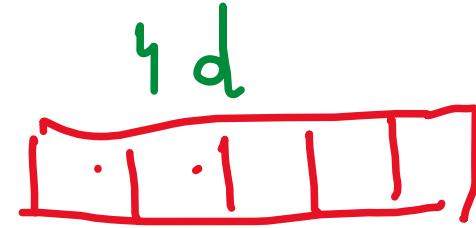
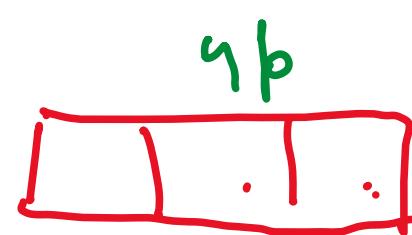
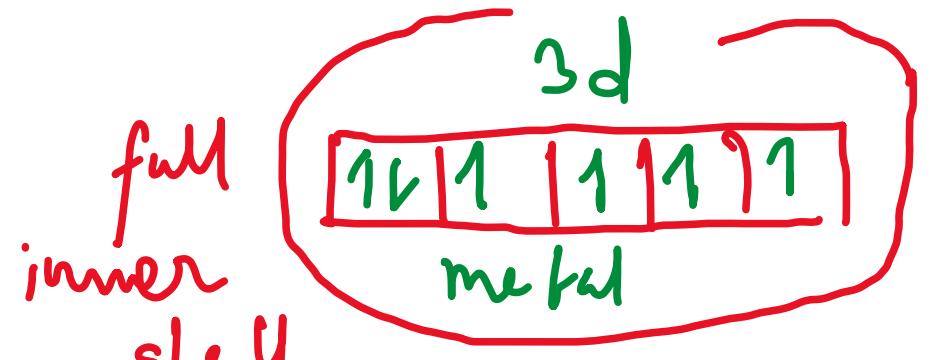
- no explanation for their electronic specificity.
- ii) The theory does not explain why magnetic property varies with temperature

In VBT, the formation of a complex may be considered as a series of hypothetical steps.



$$Z = 27$$





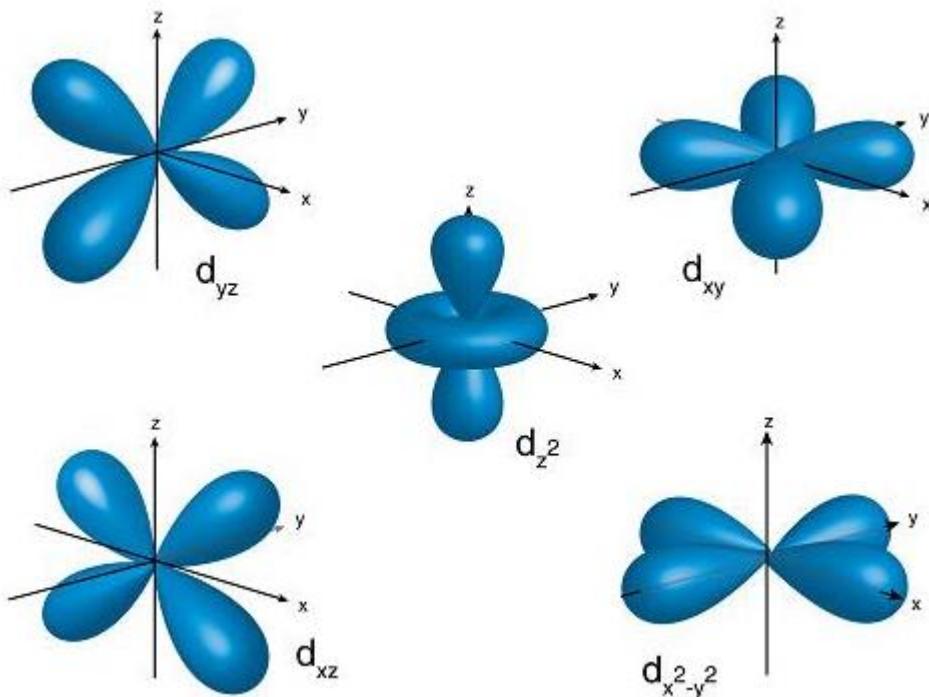
If this ion forms a complex with 6 ligands, then 6 empty atomic orbitals are required on the metal ion to receive the coordinated lone pairs of electrons. The orbitals used are the 4s, three 4p, and two 4d.

$$1s + 3p + 2d = sp^3 d^2$$



These are hybridized to give a set of 6 equivalent sp^3d^2 hybrid orbitals.

A ligand orbital containing a lone pair of electrons formed by overlapping with an empty hybrid orbital on the metal ion. In this way, a σ bond is formed with each ligand. The d orbitals used are the $4d_{xy}$ and $4d_{z^2}$.



Shape of d orbitals

High spin complex
Outer orbital complex

full inner shell $3d$

Octahedral
sheep -

$4s$ $4p$ $4d$
 (sp³ d²)
 hybridization)

Since the outer 4d orbitals are used for bonding, this is called outer orbital complex.

The energy of these complexes are quite high, so that the complexes are inactive and extremely labile.

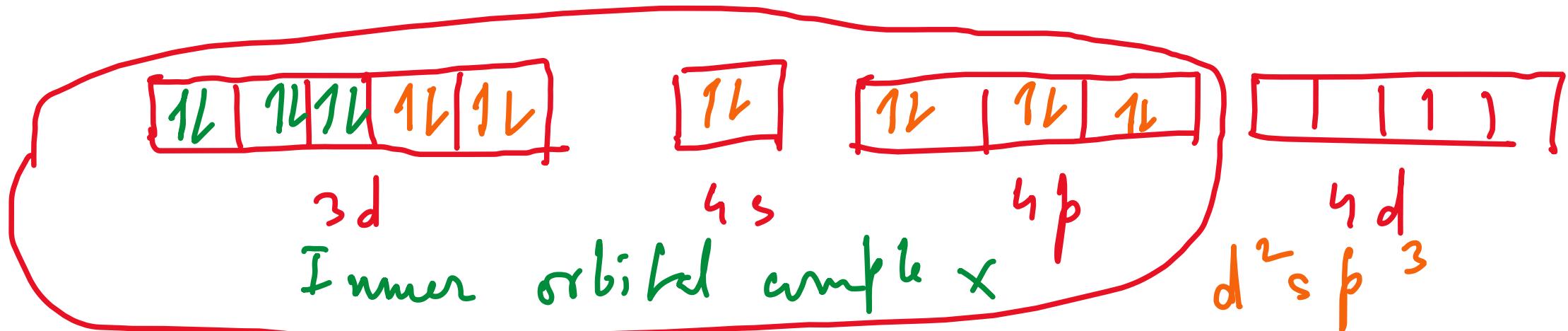
The magnetic moment depends on the no. of unpaired electrons. Because the 3d level contains the maximum no. of unpaired electrons for a

d^6 arrangement, this is sometimes called
a high-spin or spin free complex.
In Co^{3+} complex, the no. of electrons in
Metal : 6

Ligand : 12

Total electron : 18

An alternative octahedral arrangement is
possible when the electrons on the metal
ion are rearranged as shown below.



Since low energy, inner d orbitals are used this is called inner orbital complex. Such complexes are more stable than the outer orbital complexes.

Four coordinate complex.

full
inner
shell

3d

1L	1L	1L	1L	1L
----	----	----	----	----

4s

1L

4p

1L	1L	1L
----	----	----

4d

1L	1L	1L	1L
----	----	----	----

unpaired
electrons in
metal
are
forced
up.
to p. air



outer orbital form

Metals have 3d electrons.

Outer orbital form:

1L	1L	1L	1L	1L
----	----	----	----	----

1L	.
----	---

(?)

3d

J. D. Lee

Total electrons:

$$\begin{aligned} & G \times \text{Metal} + 2 \times 5 \text{ CLigand} \\ & = 6 + 8 = 14 \end{aligned}$$

4p

$dsp^2 4d$

Square Planar

1L	1L	1L
----	----	----

6 X Metal +

2 X 5 CLigand

Strong field Ligand cause the pairing
of electrons.

Strong field ligands: CO , CN^- , NO_2^- ,
 en , py , NH_3

Weak field ligands: H_2O , OH^- , F^- ,
 Cl^- , B_3O_3^- , I^-

Diamagnetic \therefore all electrons are paired.
Paramagnetic: Contains unpaired electrons.

Crystal Field Theory

Strong field ligand causes greater separation and thus results in the formation of low spin complexes by pairing of electrons.

Weak field ligands result in the formation of high spin complex.

Assumptions of CFT.

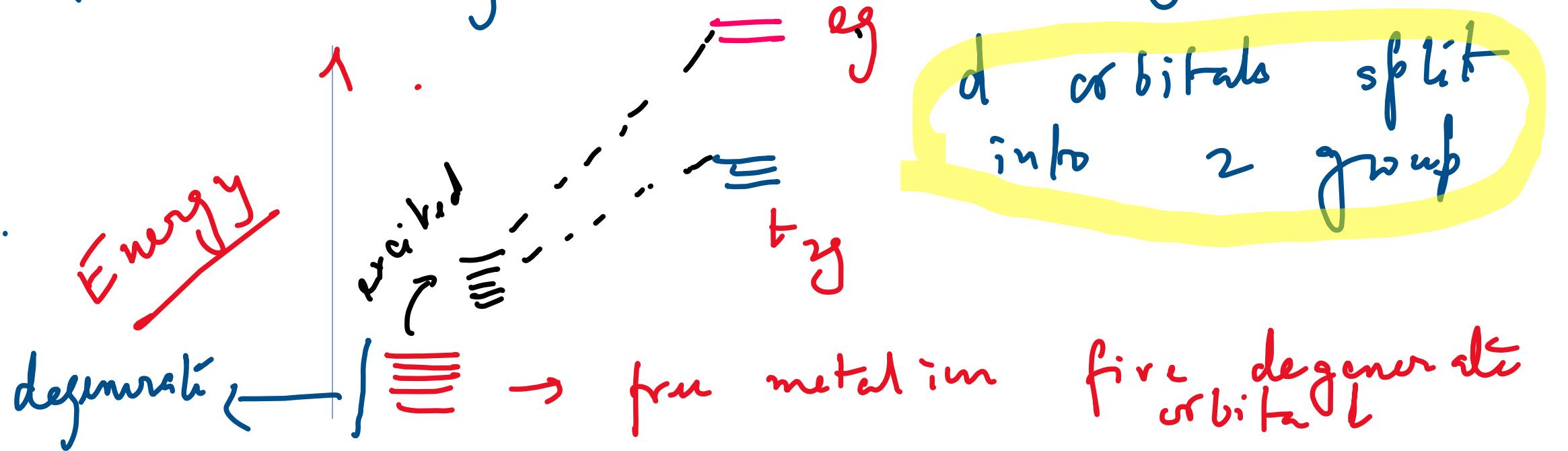
1. Ligands are considered as point charges
2. There is no interaction between metal orbitals and ligand orbitals.
3. The d orbitals on the metal all have the same energy (i.e. degenerate) in the ground state. However, when a complex is formed, the

The degeneracy is destroyed due to repulsion between the field and the electrons on the metal.

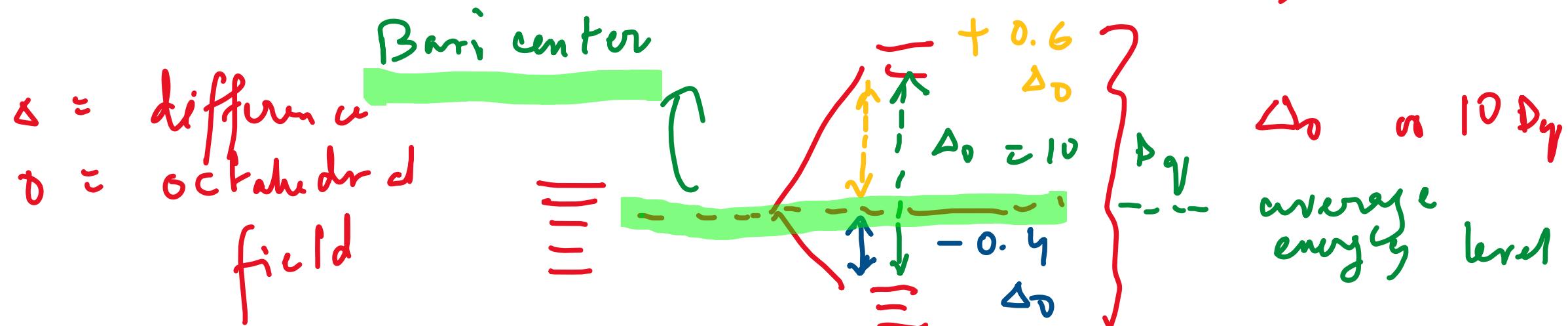
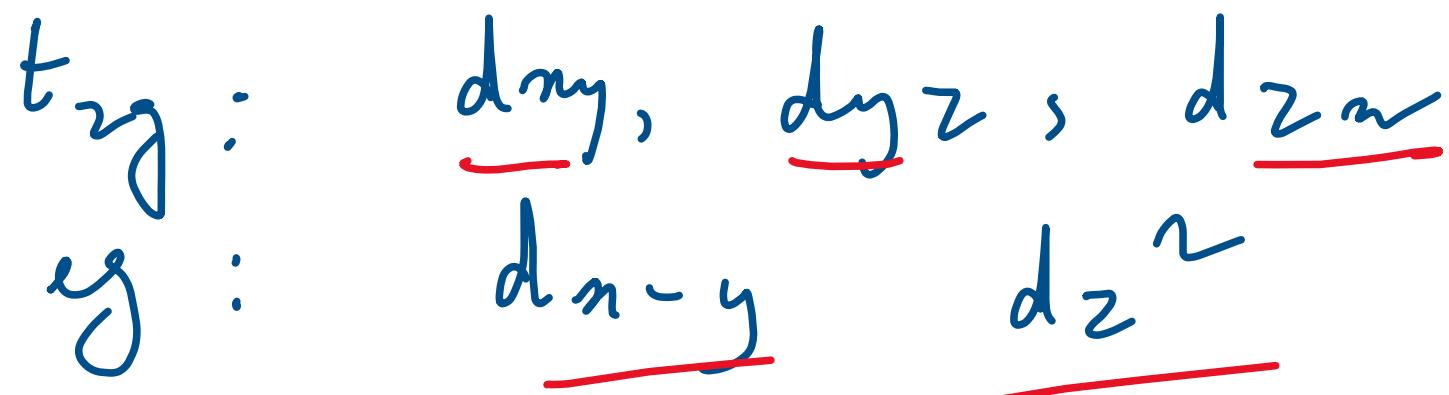
In most transition metal complex, either 6 or 4 ligands surround the metal giving rise to either octahedral or Tetrahedral structure. In both of these cases, the field produced by the ligands is

not spherically symmetrical. Thus the d orbitals are not equally affected by the ligand field.

Octahedral field: \rightarrow Crystal field splitting



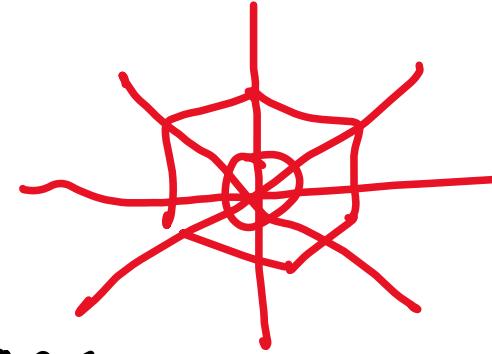
Octahedral complexes: e_g orbitals
 are of higher energy than t_{2g} orbital.



Rather than referring to the energy level of isolated metal atom, the weighted mean of the two sets of perturbed orbitals is taken as zero. This is sometimes called as Barri center.

The difference in energy between the two d levels is given either of the symbols Δ_D or $10 Dq$. It follows that the t_{2g} orbitals are $+0.6 \Delta_D$ above the energy level & $t_{1g} - 0.4 \Delta_D$ below the average.

Coordination Chemistry



$g \rightarrow$ gerade \rightarrow even

$u \rightarrow$ ungerade \rightarrow odd

German word

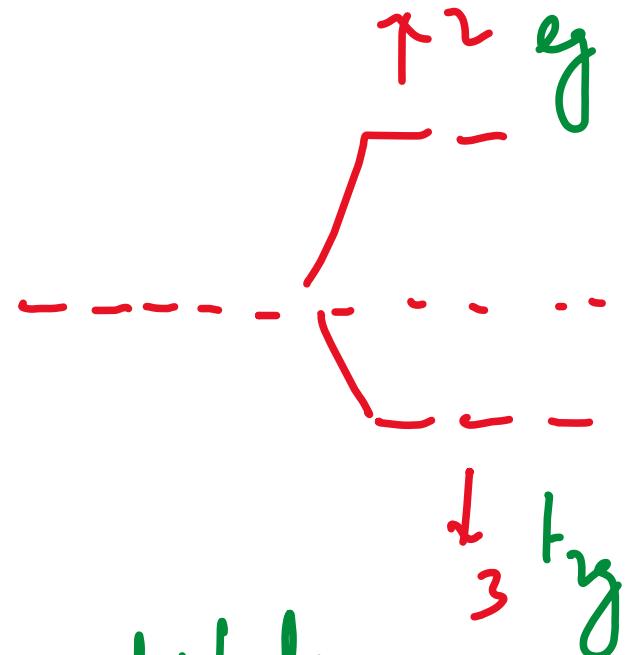
If inversion through the center of symmetry in a molecule results in the same phases for the molecular orbital, the MO is said to have

gerade symmetry -

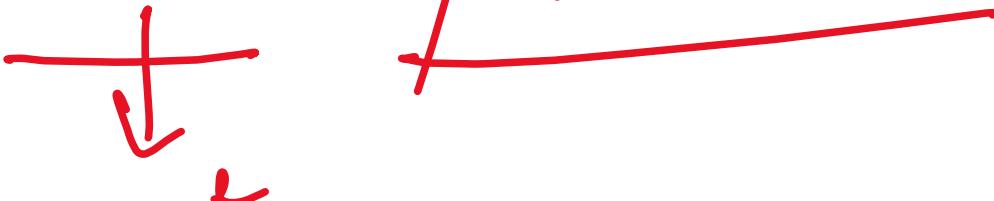
t_{2g} → "F" refers
to triply degenerate orbitals

"g" → tells us that the orbitals
are gerade - i.e. they have the same
symmetry w.r.t. the inversion center.

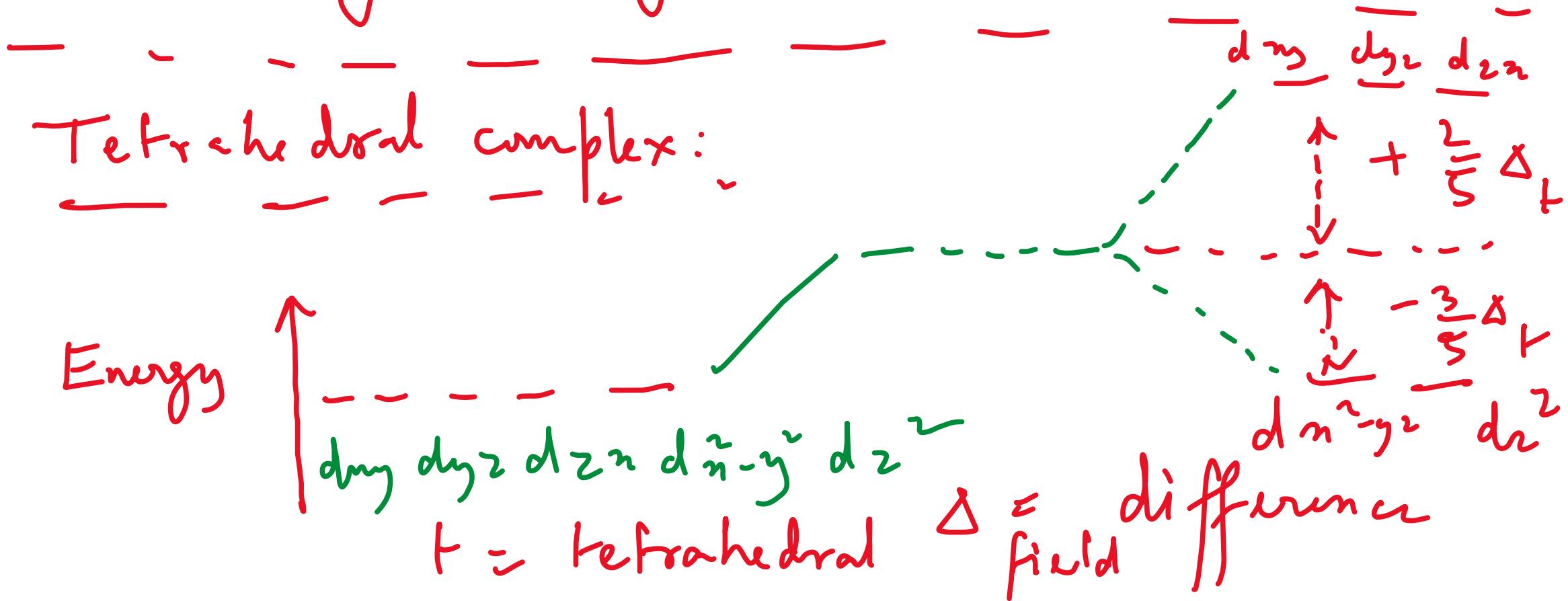
The d_{xy} , d_{xz} , d_{yz} orbitals are
collectively called t_{2g} orbitals.



eg : Excited / activated state



$g \rightarrow g_{\text{exc}}$.



Crystal Field Stabilisation Energy

C.F.S.E

The Crystal Field Stabilisation Energy is defined as the energy of the electronic configuration in the ligand field minus the energy of the electronic configuration in the isotropic field.

Factors affecting Δ_o

1. Nature of the ligands
2. Charge on the metal ion
3. Whether the metal is in the first, second, or third row of transition elements.

Spectrochemical series: A spectrochemical series is a list of ligands ordered on ligand strength and on list of metal ions

based on oxidation number, group and its identity.



Weak field

Ligands which can cause only a small degree of crystal field splitting.

Spectrochemical series (Ligands)

Experimentally determined



Strong field-

Ligands which can cause a large splitting.

Spectrochemical series :

It is difficult to explain the order as if incorporates the effect of both σ and π bonding -

Halides are in the order expected from electrostatic effects. In other case, we must consider covalent bonding to explain the order -

N.B.: Historical background.

The spectrochemical series was first proposed in 1938 based on the results of absorbing spectra of cobalt am fleses ultra violet, v.v. spectroscopy

Pattern of increasing order :-

H atoms down < o down < N down <

Spectrochemical series of metal: c down

The metal ions can also be arranged in order of increasing Δ , and this order is largely independent on the identity of ligand.



Ga chrs : (Two useful trends)

- i) Δ increases with increasing oxidation no.
- ii) Δ (I) down a group.

C. F. S. E :

System

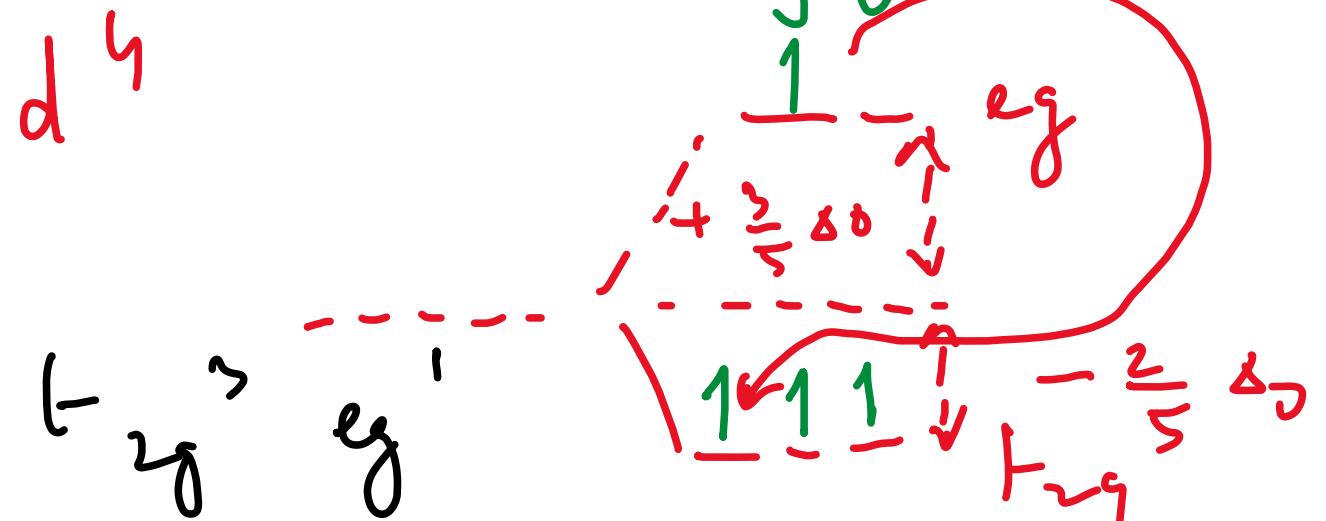
Electronic Configuration CFSE

High Spin	\longrightarrow	CFSE?
Low Spin	\longleftarrow	CFSE?

Octahedral complex

System

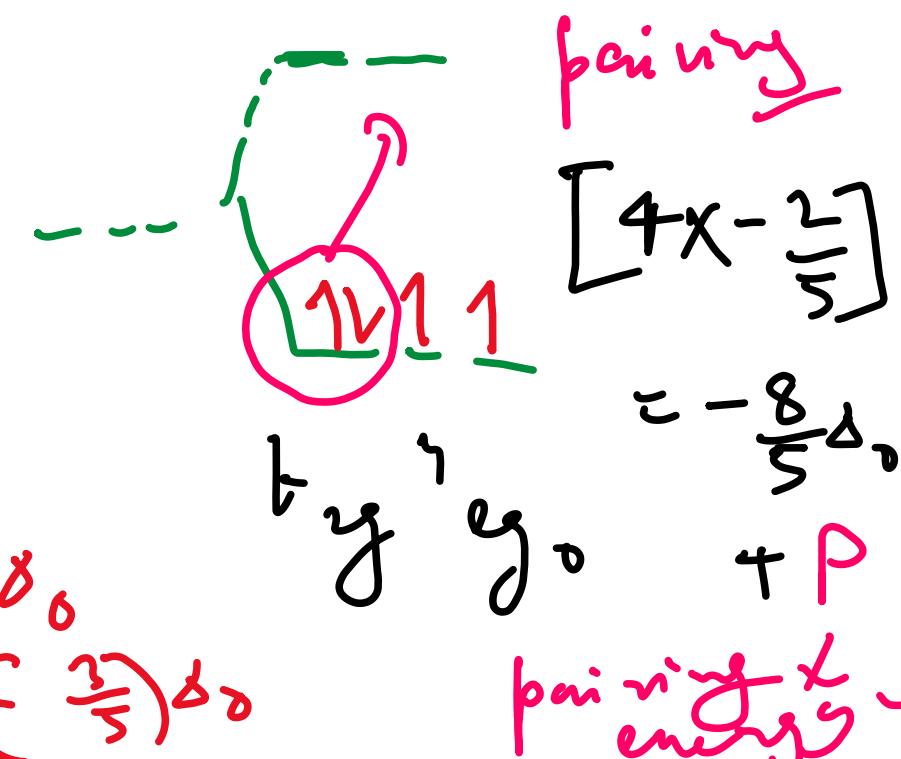
High spin
Electronic
Configuration



CFSE

Low Spin
Electronic
Configuration

CFSE

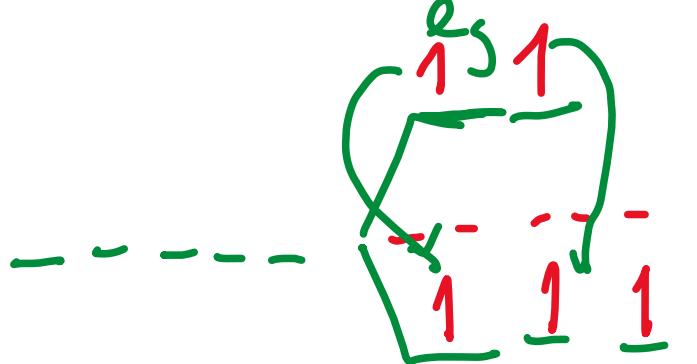


$$\text{CFSE} : \left[3 \times \left(-\frac{2}{5} \right) + \left(\frac{3}{5} \right) \right] \delta_0 = -\frac{6}{5} + \frac{3}{5} = -\left(\frac{3}{5} \right) \delta_0$$

pairing + energy

d^5 :

High Spin



$$\mu = \sqrt{S(S+1)} \\ S = \frac{5}{2}$$

Low spin

1 1 1 1 1

1 L 1 L 1

1.732

$$= \left[\frac{3 \times 2}{5} + 2 \times \frac{3}{5} \right] \Delta_0 \\ = \left[\frac{6}{5} + \frac{6}{5} = 0 \right] \Delta_0$$

Magnetic moment

$$\mu = \sqrt{n(n+1)}$$

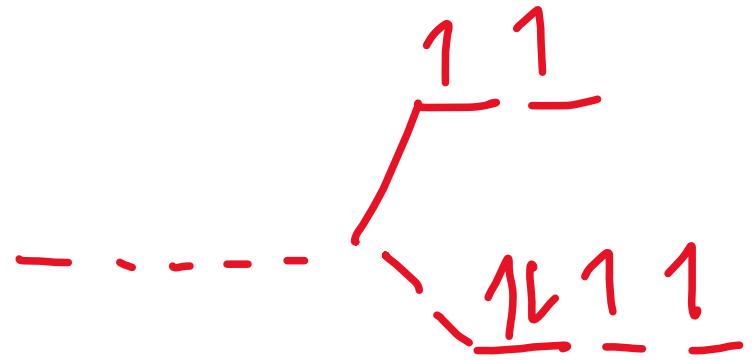
where $n = \text{no. of unpaired electrons}$

C.F.S.E :

$$= -2\Delta_0 + 2P \left[\frac{8 \times -2}{8} \right] \Delta_0$$

d^4 : High spin

$t_{2g}^4 g^2$



$$\text{C.F.S.E} = \left[-4 \times \frac{2}{5} + 2 \times \frac{3}{5} \right] \Delta_0$$

$$= -\frac{8}{5} + \frac{6}{5} = -\frac{2}{5} \Delta_0 + P$$

$$\mu = \sqrt{\gamma(\gamma+2)} = \sqrt{29}$$

Low spin

$t_g^4 e_g^2$

$$\begin{aligned} \text{C.F.S.E} &= -Cx \frac{2}{5} \\ &= -\frac{12}{5} \Delta_0 \\ &\quad + 3P \end{aligned}$$

$$\mu = \sqrt{0}$$

$$= D \Rightarrow$$

paramagnetic

d^7 :

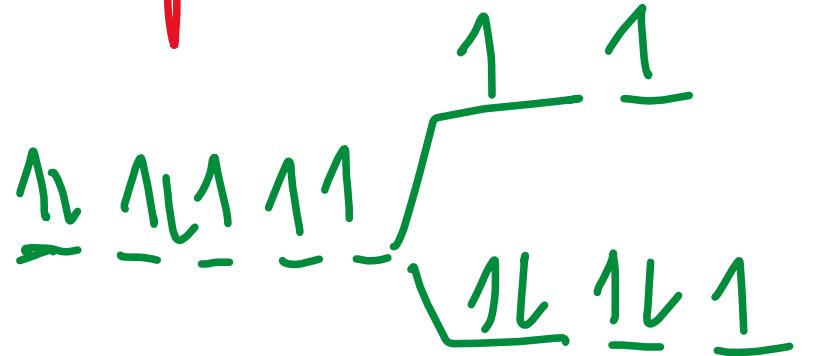
High Spin

Electronic

Configuration

C.F.S.E

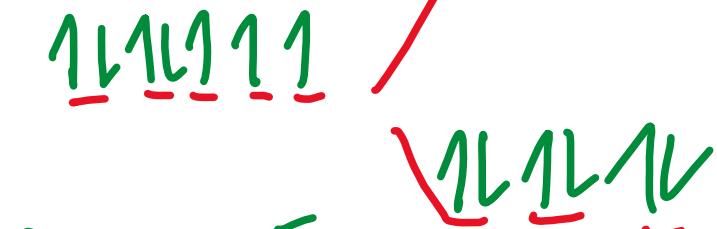
Magnetic moment.



$$C.F.S.E = \left[5 \times \frac{2}{5} + 2 \times \frac{3}{5} \right] \Delta_0$$

$$\mu = \sqrt{5(3+2)} \cdot t_{2g}^5 g_J = \sqrt{15} = 3.87 D$$

Low Spin



$$C.F.S.E = -6 \times \frac{2}{5} + 1 \times \frac{3}{5}] \Delta_0$$

$$= -\frac{9}{5} \Delta_0 +$$

$$t_{2g}^6 eg^1 3P^-$$

$$\mu = \sqrt{3} \Delta_0$$

Practical application -

C. F. S. E & } pairing energy } of some complexes {

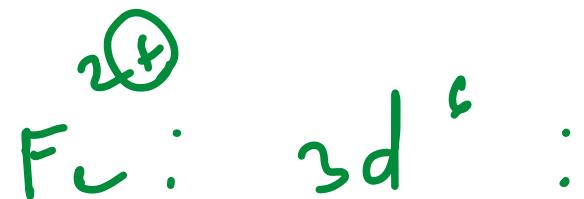
$- 4 \times \frac{2}{5} + 2 \times \frac{3}{5}$

$- \frac{8}{5} + \frac{6}{5}$

$= - \frac{2}{5}$

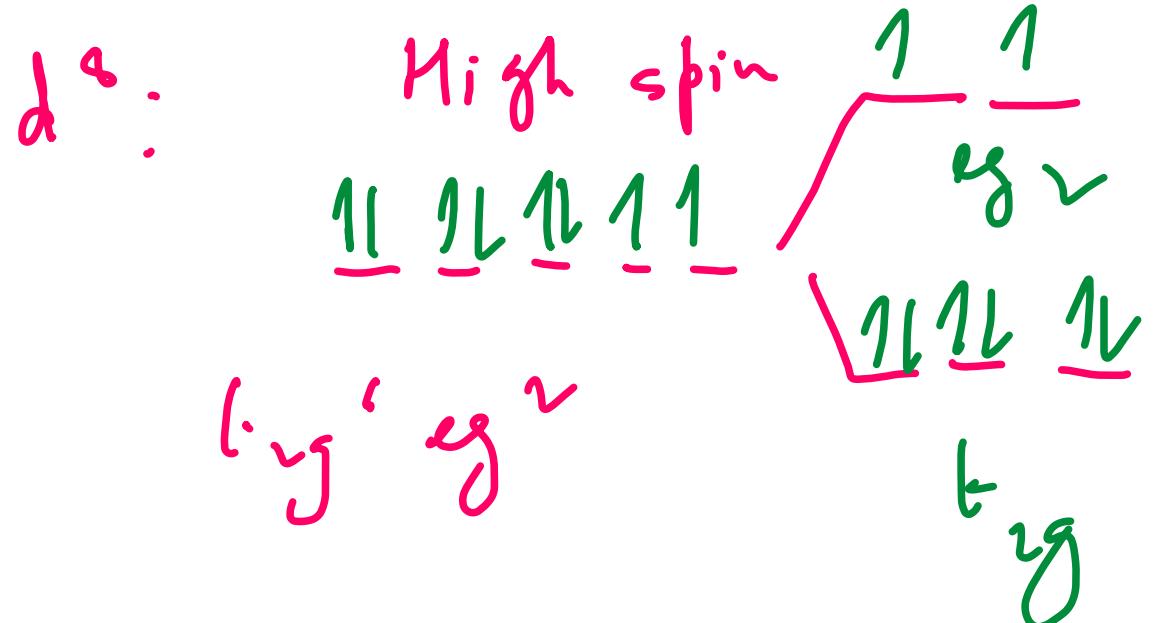
$\left[\text{Fe}(\text{H}_2\text{O})_6 \right]^{2+}$

1. Calculate the oxidation state.
2. Whether the ligand is strong or weak.
3. Write the electronic configuration.
4. Calculate C. F. S. E.



$$\begin{array}{ccccccc}
 & & & & & & \\
 & 1 & 1 & 1 & 1 & 1 & \\
 & \diagdown & \diagup & \diagdown & \diagup & \diagdown & \\
 & 1 & 1 & 1 & 1 & 1 & \\
 \end{array}$$

$[-4 \times 0.4 + 2 \times 0.6]$
 $= -1.6 + 1.2 = 0.4 \text{ OAO}$



$$C.F.S.E : \left[-\frac{2}{5} \times 6 + \frac{3}{5} \times 2 \right] \delta_0$$

$$= -\frac{12}{5} + \frac{6}{5} = -\frac{6}{5} \delta_0$$

$$= -\frac{6}{5} \delta_0 + 3 P$$

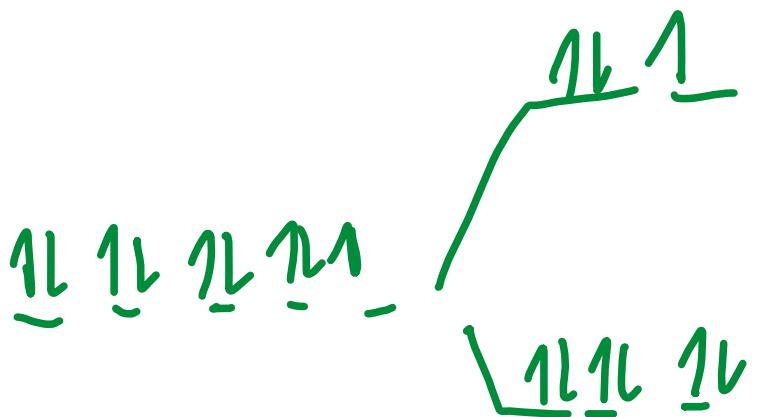
$$\lambda = \sqrt{n(2+2)} = \sqrt{8} = 2.83$$

Low spin:

t_{2g}, e_g

\therefore The t_{2g} level is completely filled

d^9 :



$t_{2g}^4 e_g^3$

$$C.F.S.E = -\frac{3}{5} \Delta_D + 4P$$

$$\begin{aligned} h &= \sqrt{1(1+2)} = \sqrt{3} \\ &= 1.732 \end{aligned}$$

Low spin =

High spin

(in all respects)

d^{10} : $t_{2g}^5 e_g^5$

$C.F.S.E$: $0 + 5P$

Tetrahedral Complex

$$d^4 : e_g^2 t_{2g}^2 \quad C.F.S.E. : \left(2x - \frac{3}{5} + 2x \frac{2}{5} \right) \Delta_T \\ = -\frac{2}{5} \Delta_T$$

High spin

Low spin:

$$e_g^4 t_{2g}^0 : C.F.S.E : 4x - \frac{3}{5}$$

~~Q~~; amagnetic moment:

$$\lambda = \sqrt{4(9+2)} = \sqrt{24} = 4.9.$$

$$= -\frac{12}{5} \Delta_L + 2P^o$$

d^5 : High spin: $t_{2g}^2 t_{xy}^3$: C.F.S.E. = 0

Low spin

$t_{2g}^5 t_{xy}^1$

$$-2\Delta_F + 2\delta$$

Magnetic moment: $\sqrt{5\alpha\gamma}$

$$\mu \approx \sqrt{3} = 1.732\mu_D$$

$$= \sqrt{35} = 5.92\mu_D$$

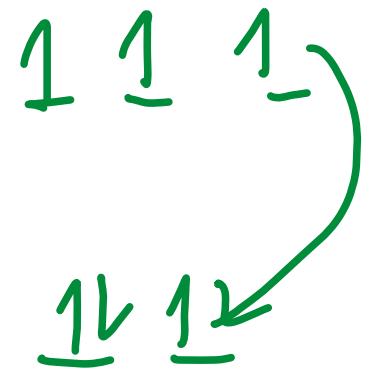
d^6 : High spin: $t_{2g}^3 t_{xy}^3$

"

$t_{2g}^4 t_{xy}^2$

C.F.S.E: High spin:

$$(-\frac{3}{2}) \Delta_F + P$$



Low spin:

$$-\frac{8}{5} \Delta_F + 2P$$

Magnetic moment:

High spin:

$$\sqrt{4C_4 + 2}$$

Low spin

$$\sqrt{2(2+2)}$$

$$\begin{aligned} &= \sqrt{2g} \\ &= \sqrt{8} \\ &\approx 2.8 > D \end{aligned}$$

Take home message —

Crystal field theory (C.C.F.T) is a bonding model that explains many important characteristics of coordination compounds/ transition metal complexes, including the —

- i.) Color
- ii.) Magnetism
- iii.) Structure
- iv.) Stability
- v.) Reactivity

Knowing the color can have a

W. o f useful applications - such
as creating of pigments for
dyes in the textile industry -

Color

Ligand to metal
charge transfer -

d-d transition

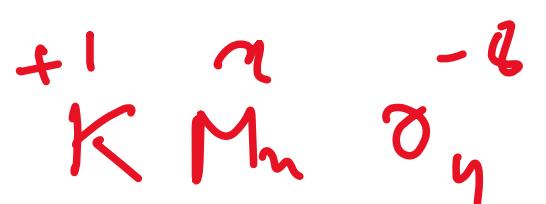
Electron transition between
split d-orbital energy levels

Gem Stones

Ruby,
emerald

Potassium permanganate is colored because it absorbs light in the visible range of the electro magnetic spectrum.

Source of color: Ligand to metal charge transfer takes place between the oxygen's p orbitals and vacant d orbitals of metal.



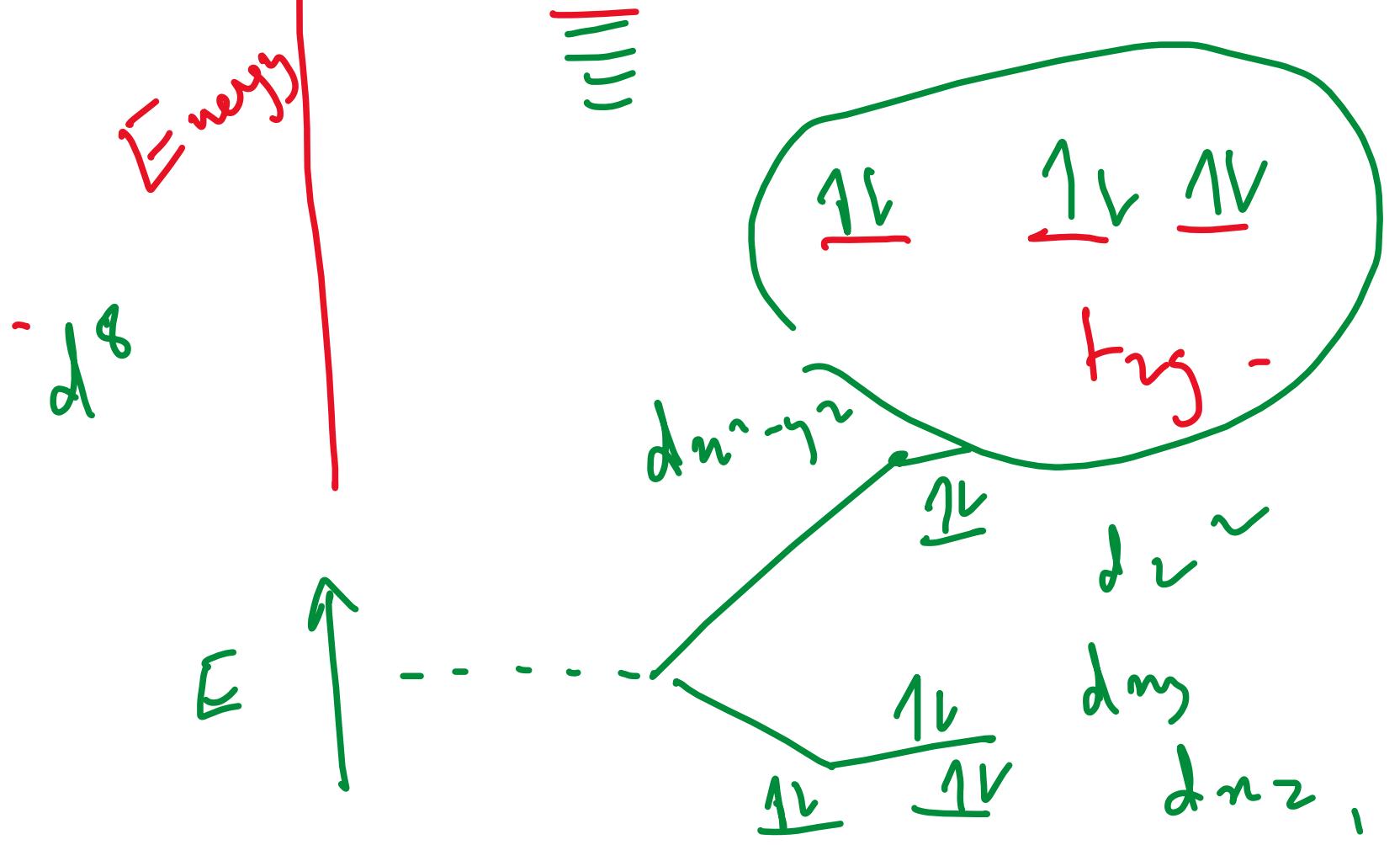
D.S. : 7

$$n - 7 = 2 \Rightarrow n = 7$$

Mn(VII) : d orbital of the central metal atom is empty.

Thus charge transfer occurs from p orbitals of O to empty d orbitals of metal leading to an intense pink/violet colouration.

Tetragonal distortion - $d_{z^2} - g_2$
 $\cong d_{z^2}$.



Tetragonal distortion splits the eg level in very strong octahedral field.

Square planar complexes are formed by d^8 ions with strong field ligands.



weak field

2^+

strong field -

$Sp^3 \rightarrow$
Tetrahedral

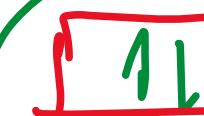


strong field

$3d$



Sq are



$4s$



$4p^-$

d^8
 $[Ni^{II}(CN)_4]$

Planar

