

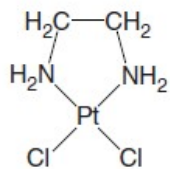
# Coordination Compounds

- A coordination compound is any compound that contains a coordination entity
- A coordination entity is an ion or neutral molecule: composed of a **central metal atom** to which is attached a surrounding array of other **atoms or groups of atoms**, each of which is called a ligand.

# Coordination Compounds

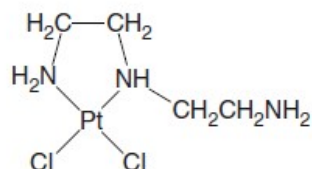
- **Coordination number**: the number of  $\sigma$ -bonds between ligands and the central atom.
- **Chelation**: coordination of more than one non-contiguous  $\sigma$ -electron pair donor atom from a given ligand to the same central atom.

1.



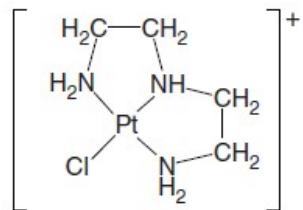
bidentate chelation

2.



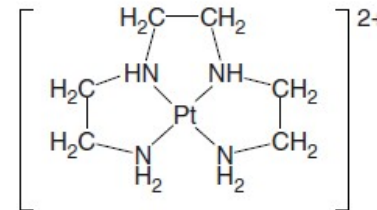
bidentate chelation

3.



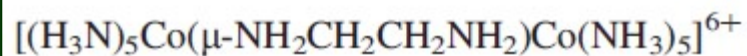
tridentate chelation

4.



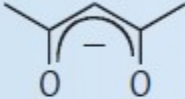
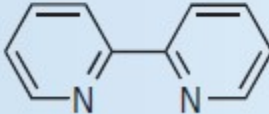
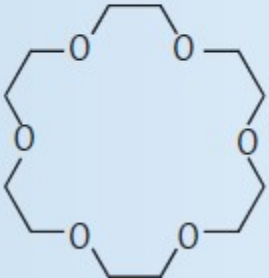
tetradentate chelation

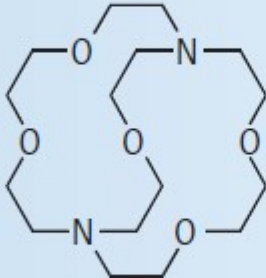
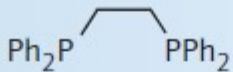
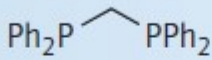
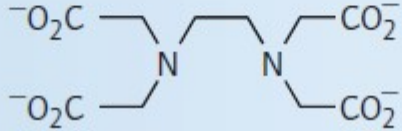
## Chelating vs Bridging

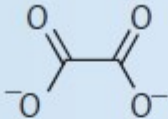
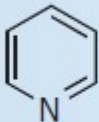
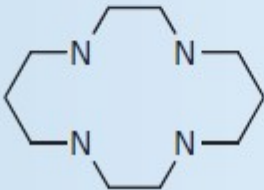


# Oxidation State

	<i>Formula</i>	<i>Ligands</i>	<i>Central atom oxidation state</i>
1.	$[\text{Co}(\text{NH}_3)_6]^{3+}$	6 $\text{NH}_3$	III
2.	$[\text{CoCl}_4]^{2-}$	4 $\text{Cl}^-$	II
3.	$[\text{MnO}_4]^-$	4 $\text{O}^{2-}$	VII
4.	$[\text{MnFO}_3]$	3 $\text{O}^{2-}$ + 1 $\text{F}^-$	VII
5.	$[\text{Co}(\text{CN})_5\text{H}]^{3-}$	5 $\text{CN}^-$ + 1 $\text{H}^-$	III
6.	$[\text{Fe}(\text{CO})_4]^{2-}$	4 $\text{CO}$	-II

Name	Formula	Abbreviation	Donor atoms	Number of donors
Acetylacetonato		acac <sup>-</sup>	O	2
Ammine	NH <sub>3</sub>		N	1
Aqua	H <sub>2</sub> O		O	1
2,2-Bipyridine		bpy	N	2
Bromido	Br <sup>-</sup>		Br	1
Carbanato	CO <sub>3</sub> <sup>2-</sup>		O	1 or 2
Carbonyl	CO		C	1
Chlorido	Cl <sup>-</sup>		Cl	1
1,4,7,10,13,16-Hexaoxa-cyclooctadecane		18-crown-6	O	6

Name	Formula	Abbreviation	Donor atoms	Number of donors
4,7,13,16,21-Pentaoxa-1,10-diaza-bicyclo[8.8.5]tricosane		2.2.1 crypt	N, O	2N, 5O
Cyanido	CN <sup>-</sup>		C	1
Diethylenetriamine	NH(CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ) <sub>2</sub>	dien	N	3
Bis(diphenylphosphino)ethane		dppe	P	2
Bis(diphenylphosphino)methane		dppm	P	2
Cyclopentadienyl	C <sub>5</sub> H <sub>5</sub> <sup>-</sup>	Cp <sup>-</sup>	C	5
Ethylenediamine (1,2-diaminoethane)	NH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	en	N	2
Ethylenediaminetetraacetato		edta <sup>4-</sup>	N, O	2N, 4O

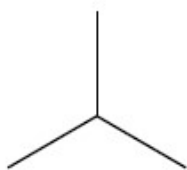
Fluorido	$F^-$		F	1
Glycinato	$NH_2CH_2CO_2^-$	gly	N, O	1N, 1O
Hydrido	$H^-$		H	1
Hydroxido	$OH^-$		O	1
Iodido	$I^-$		I	1
Nitrato	$NO_3^-$		O	1 or 2
Nitrito – $\kappa O$	$NO_2^-$		O	1
Nitrito – $\kappa N$	$NO_2^-$		N	1
Oxido	$O^{2-}$		O	1
Oxalato		ox	O	2
Pyridine		py	N	1
Sulfido	$S^{2-}$		S	1
Tetraazacyclotetradecane		cyclam	N	4

Thiocyanato— $\kappa N$	$\text{NCS}^-$		N	1
Thiocyanato— $\kappa S$	$\text{SCN}^-$		S	1
Thiolato	$\text{RS}^-$		S	1
Triaminotriethylamine	$\text{N}(\text{CH}_2\text{CH}_2\text{NH}_2)_3$	tren	N	4
Tricyclohexylphosphine	$\text{P}(\text{C}_6\text{H}_{11})_3$	$\text{PCy}_3$	P	1
Trimethylphosphine	$\text{P}(\text{CH}_3)_3$	$\text{PMe}_3$	P	1
Triphenylphosphine	$\text{P}(\text{C}_6\text{H}_5)_3$	$\text{PPh}_3$	P	1

# Coordination number and geometry

## Three-coordination

trigonal plane



*TP-3*

trigonal pyramid



*TPY-3*

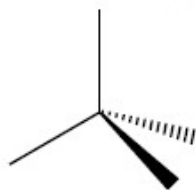
T-shape



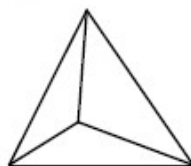
*TS-3*

## Four-coordination

tetrahedron



*T-4*



square plane



*SP-4*



square pyramid



*SPY-4*

see-saw



*SS-4*

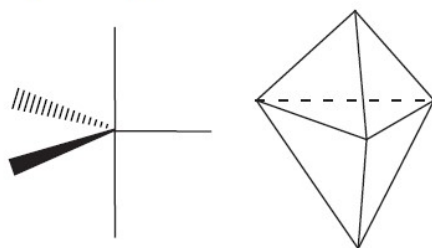




# Coordination number and geometry

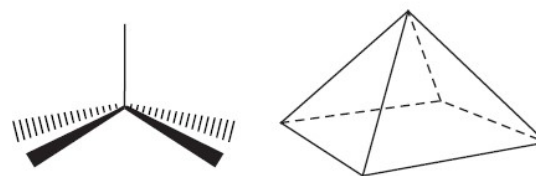
## *Five-coordination*

trigonal bipyramid



*TBPY-5*

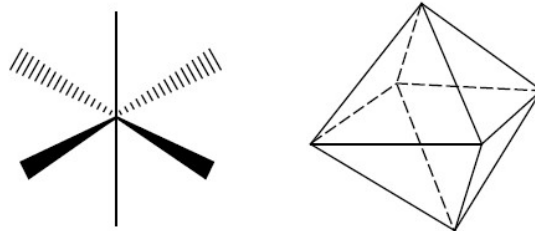
square pyramid



*SPY-5*

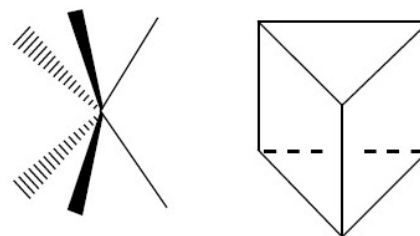
## *Six-coordination*

octahedron



*OC-6*

trigonal prism

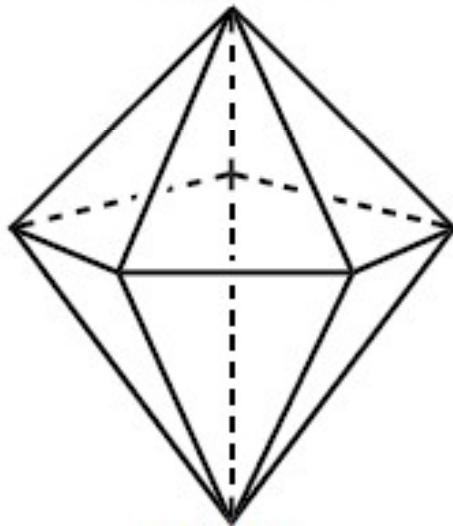


*TPR-6*

# Coordination number and geometry

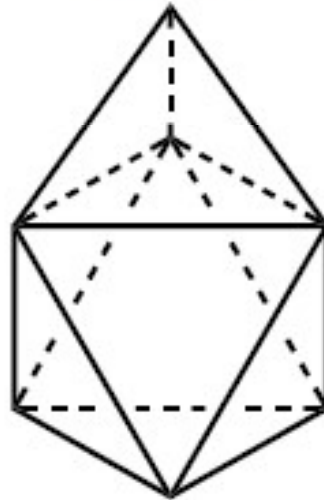
*Seven-coordination*

pentagonal  
bipyramid



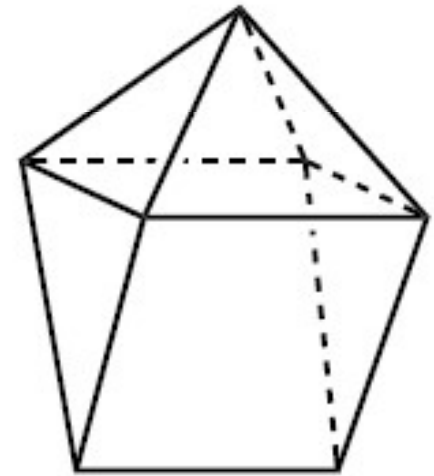
*PBPY-7*

octahedron, face  
monocapped



*OCF-7*

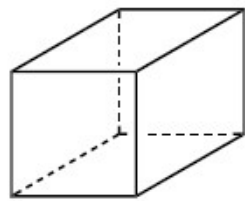
trigonal prism,  
square-face monocapped



*TPRS-7*

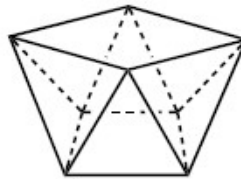
# Coordination number and geometry

*Eight-coordination*  
cube



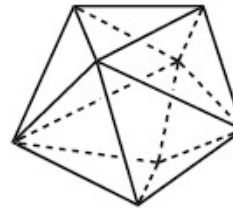
*CU-8*

square  
antiprism



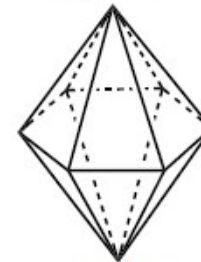
*SAPR-8*

dodecahedron



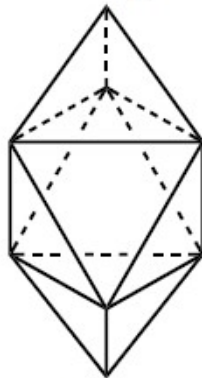
*DD-8*

hexagonal  
bipyramid



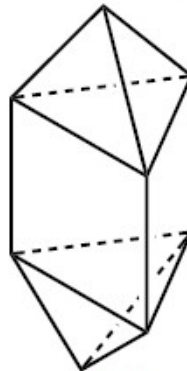
*HBPY-8*

octahedron,  
*trans*-bicapped



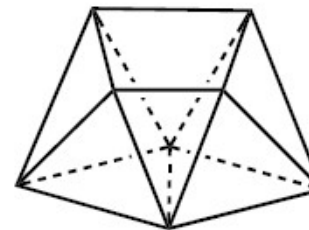
*OCT-8*

trigonal prism,  
triangular-face bicapped



*TPRT-8*

trigonal prism,  
square-face bicapped

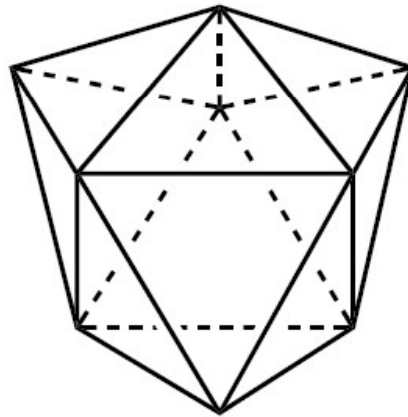


*TPRS-8*

# Coordination number and geometry

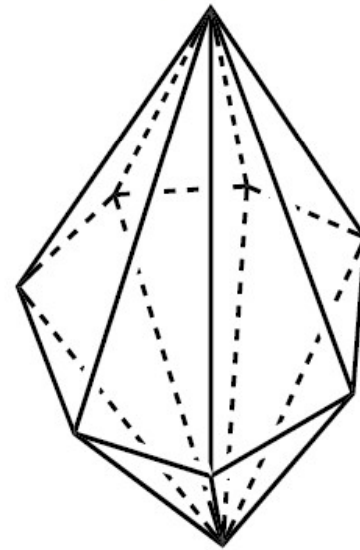
*Nine-coordination*

trigonal prism,  
square-face tricapped



*TPRS-9*

heptagonal  
bipyramid



*HBPY-9*

# Coordination nomenclature: an additive nomenclature

*Example:*

1. Addition of ligands to a central atom:

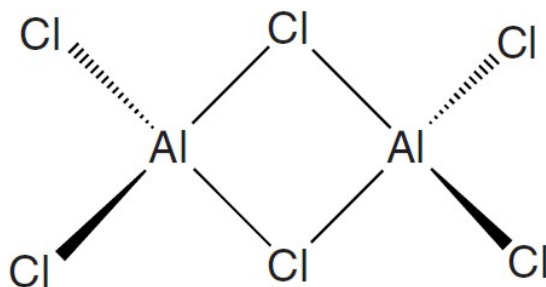


Addition of ligand names to a central atom name:

hexaaquanickel(II)

# Bridging Ligands

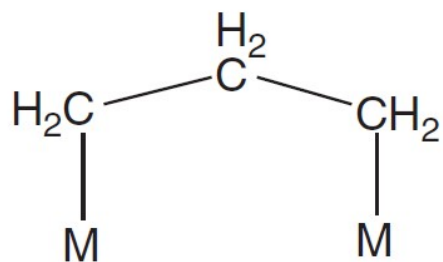
- Form polynuclear species
- $\mu$  as a prefix to the ligand formula or name
  - The number of central atoms joined into a single coordination entity by bridging ligands: indicated by using the terms dinuclear, trinuclear, tetranuclear, etc



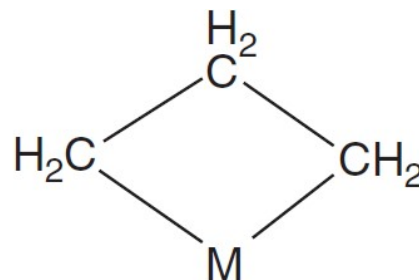
di- $\mu$ -chlorido-tetrachlorido- $1\kappa^2\text{Cl}, 2\kappa^2\text{Cl}$ -dialuminium

# Bridging Ligands

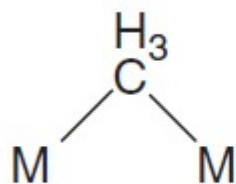
- mu ( $\mu$ ) convention



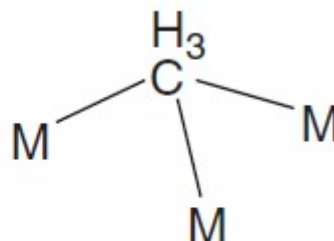
$\mu$ -propane-1,3-diyl  
(bridging)



propane-1,3-diyl  
(chelating)



$\mu$ -methyl



$\mu_3$ -methyl

# Metal–metal bonds

1.  $[\text{Br}_4\text{ReReBr}_4]^{2+}$   
bis(tetrabromidorhenium)(*Re*—*Re*)(2+)



# Naming Coordination Compounds

- ligand names are listed before the name(s) of the central atom(s)
- **no spaces** are left between parts of the name that refer to the same coordination entity,
- **ligand names** are listed in **alphabetical order** (multiplicative prefixes indicating the number of ligands are not considered in determining that order),
- the use of **abbreviations** in names is **discouraged**.
- Names of **anionic coordination entities** are furthermore given the ending **‘ate’**.



penta**a**mmine**c**hloridocobalt(2+) chloride



tetraxenonidogold(2+)

# Number of ligands

- Two kinds of multiplicative prefix are available
  - Prefixes **di, tri, etc.** are generally used with the names of **simple ligands**. Enclosing marks are not required.
  - Prefixes **bis, tris, tetrakis**, etc. are used with **complex ligand names** and in order to avoid ambiguity. **Enclosing marks must be placed around the multiplicand.**
  - **diammine for  $(\text{NH}_3)_2$ , but bis(methylamine)**

# Representing ligands in names

- Names of anionic ligands,, are modified to end in 'o'.
- In general, if the anion name ends in 'ide', 'ite' or 'ate', the final 'e' is replaced by 'o', giving 'ido', 'ito' and 'ato', respectively.
  - In particular, alcoholates, thiolates, phenolates, carboxylates, partially dehydronated amines, phosphanes, etc. are in this category.
- neutral and cationic ligands, including organic ligands, are used without modification
- Enclosing marks are required for
  - neutral and cationic ligand names,
  - for names of inorganic anionic ligands containing multiplicative prefixes (such as triphosphato), for compositional names (such as carbon disulfide),
  - for names of substituted organic ligands
- Ligands binding to metals through carbon atoms to be discussed in organometallic compounds

# Examples

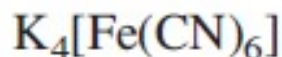
<i>Formula</i>	<i>Ligand name</i>
1. $\text{Cl}^-$	chlorido
2. $\text{CN}^-$	cyanido
3. $\text{H}^-$	hydrido <sup>3</sup>
4. $\text{D}^-$ or $^2\text{H}^-$	deuterido <sup>3</sup> or [ <sup>2</sup> H]hydrido <sup>3</sup>
5. $\text{PhCH}_2\text{CH}_2\text{Se}^-$	2-phenylethane-1-selenolato
6. $\text{MeCOO}^-$	acetato or ethanoato
7. $\text{Me}_2\text{As}^-$	dimethylarsanido
8. $\text{MeCONH}_2$	acetamide ( <i>not</i> acetamido)
9. $\text{MeCONH}^-$	acetylazanido or acetylamido ( <i>not</i> acetamido)
10. $\text{MeNH}_2$	methanamine

# Examples

- |                         |  |
|-------------------------|--|
| 11. $\text{MeNH}^-$     | methylazanido, or methylamido, or methanaminido<br>( <i>cf.</i> Example 3 of Section IR-6.4.6) |
| 12. $\text{MePH}_2$     | methylphosphane  |
| 13. $\text{MePH}^-$     | methylphosphanido  |
| 14. $\text{MeOS(O)OH}$  | methyl hydrogen sulfite  |
| 15. $\text{MeOS(O)O}^-$ | methyl sulfite, or methanolatodioxidosulfato(1–)   |

# Charge numbers and oxidation numbers

- The oxidation number of the central atom: a **Roman numeral** appended in parentheses to the central atom name (including the ending 'ate', if applicable)
- **Arabic zero** indicates the oxidation number zero.
- Alternatively, the charge on a coordination entity may be indicated.
- The net charge is written in arabic numbers, with the number preceding the charge sign, and enclosed in parentheses.
- It follows the name of the central atom (including the ending 'ate', if applicable) without the intervention of a space.



potassium hexacyanidoferrate(II), or  
potassium hexacyanidoferrate(4-), or  
tetrapotassium hexacyanidoferrate



hexaamminecobalt(III) chloride



pentaamminechloridocobalt(2+) chloride

# Formulae of coordination compounds

- A (line) formula of a compound: provides basic information about the constitution of the compound in a concise and convenient manner
  - The central atom symbol(s) is (are) listed first
  - The ligand symbols are then listed in alphabetical order
    - Thus,  $\text{CH}_3\text{CN}$ ,  $\text{MeCN}$  and  $\text{NCMe}$  would be ordered under C, M and N respectively, and  $\text{CO}$  precedes  $\text{Cl}$  because single letter symbols precede two letter symbols.

# Formulae of coordination compounds

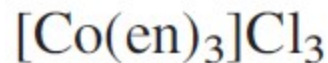
- Use of enclosing marks
  - Square brackets: formula for the entire coordination entity, whether charged or not
  - Parentheses: polyatomic ligands formulae and abbreviations of ligands.



sodium amminebromidochloridonitrito- $\kappa$ N-platinate(1–)



hexakis(methyl isocyanide)iron(II) bromide



tris(ethane-1,2-diamine)cobalt(III) trichloride



# Ionic charges and oxidation numbers

- If the formula of a charged coordination entity is to be written without that of any counterion, the charge is indicated outside the square bracket as a right superscript, with the number before the sign.
- The oxidation number of a central atom may be represented by a Roman numeral, which should be placed as a right superscript on the element symbol.
  1.  $[\text{PtCl}_6]^{2-}$
  2.  $[\text{Cr}(\text{OH}_2)_6]^{3+}$
  3.  $[\text{Cr}^{\text{III}}(\text{NCS})_4(\text{NH}_3)_2]^-$
  4.  $[\text{Cr}^{\text{III}}\text{Cl}_3(\text{OH}_2)_3]$
  5.  $[\text{Fe}^{-\text{II}}(\text{CO})_4]^{2-}$

# Specifying donor atoms

- only cases where specification of the donor atom is not required for a ligand that can bind to a central atom in more than one way
  - monodentate O-bound carboxylate groups
  - monodentate C-bound cyanide (ligand name ‘cyanido’)
  - monodentate C-bound carbon monoxide (ligand name ‘carbonyl’)
  - monodentate N-bound nitrogen monoxide (ligand name ‘nitrosyl’).

# Specifying donor atoms

- The kappa convention
  - Single ligating atoms are indicated by the italicized element symbol preceded by a Greek kappa,  $\kappa$
  - $\kappa$  placed after the portion of the ligand name that represents the ring, chain or substituent group in which the ligating atom is found



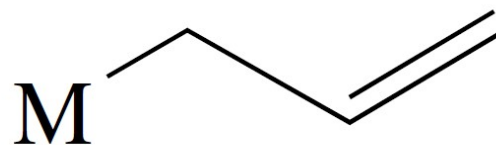
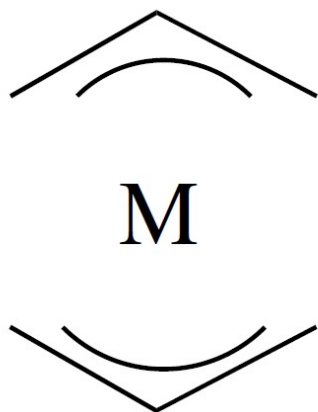
dibromido[ethane-1,2-diylbis(dimethylphosphane- $\kappa P$ )]nickel(II)

# Specifying donor atoms

- The kappa convention
  - thiocyanato- $\kappa N$  for nitrogen-bonded NCS
  - thiocyanato-  $\kappa S$  for sulfur-bonded NCS.
  - Nitrogen-bonded nitrite is named nitrito- $\kappa N$
  - Oxygen-bonded nitrite is named nitrito- $\kappa O$ , as in pentaamminenitrito-  $\kappa O$  -cobalt(III)

# Specifying donor atoms

- The eta ( $\eta$ ) convention: ('hapticity')
  - applied in cases where contiguous donor atoms within a given ligand are involved in bonding to a central atom

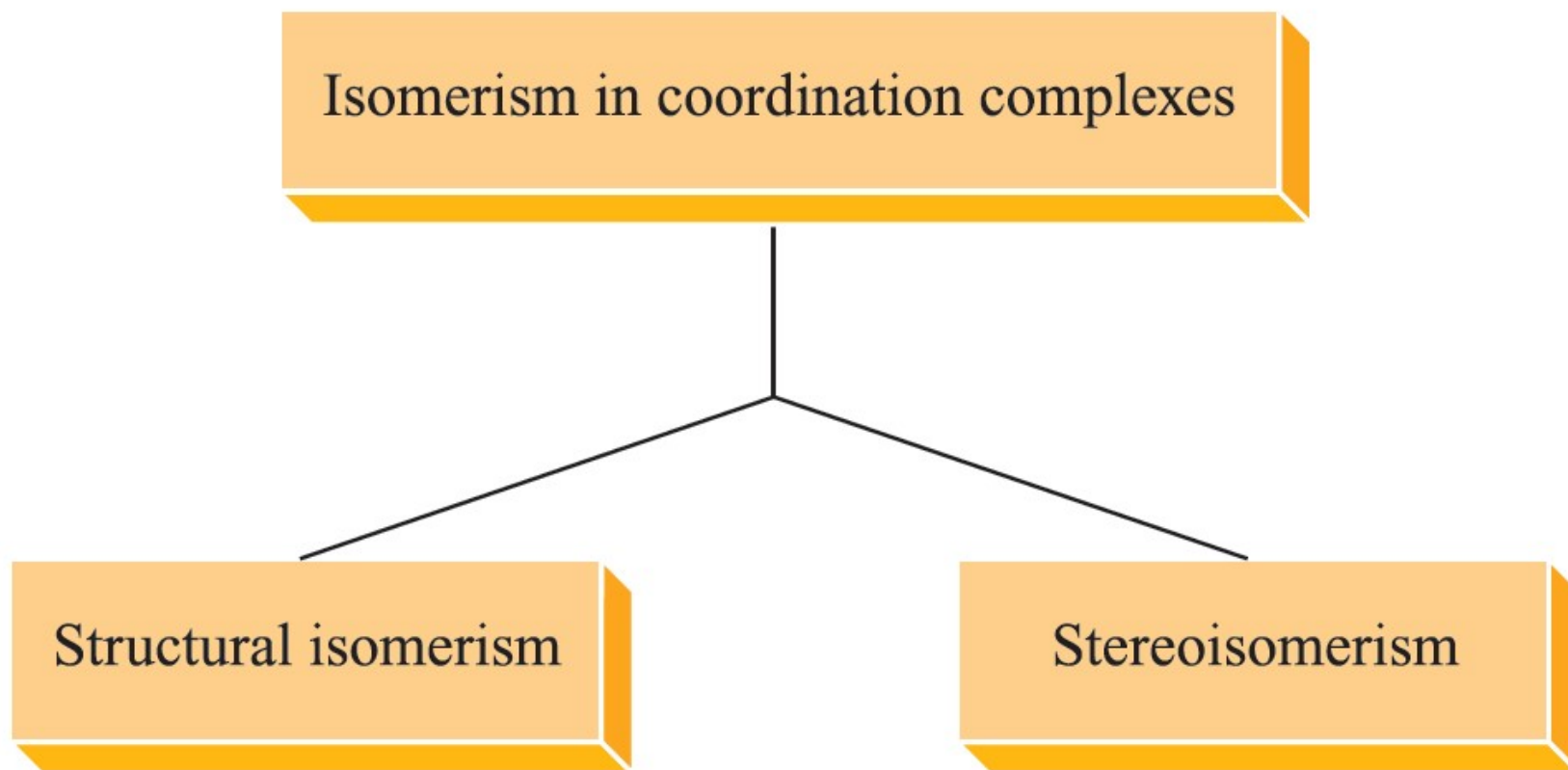


**2 electron donor and anionic**

bis- $\eta^3$ -allyl nickel, or  $[\text{Ni}(\eta^3\text{-C}_3\text{H}_5)_2]$

**4 electron donor and anionic**

# Isomerism in coordination complexes



# Isomerism in coordination complexes

Structural isomerism



```
graph TD; A[Isomerism in coordination complexes] --> B[Structural isomerism]; A --> C[Stereoisomerism]; B --> D[Ionization isomerism]; B --> E[Hydration isomerism]; B --> F[Coordination isomerism]; B --> G[Linkage isomerism]; B --> H[Polymerization isomerism]; C --> I[Geometrical isomerism]; C --> J[Optical isomerism];
```

Stereoisomerism

Ionization isomerism  
Hydration isomerism  
Coordination isomerism  
Linkage isomerism  
Polymerization isomerism

Geometrical isomerism  
Optical isomerism

# Structural isomerism: ionization isomers

- Ionization isomers result from the interchange of an anionic ligand within the first coordination sphere with an anion outside the coordination sphere.
  - violet  $[\text{Co}(\text{NH}_3)_5\text{Br}]\text{SO}_4$  and red  $[\text{Co}(\text{NH}_3)_5(\text{SO}_4)]\text{Br}$
  - The isomers are also easily distinguished by IR spectroscopy;
    - free and coordinated sulfate ions give rise to one or three IR active SO stretching vibrations respectively



# Structural isomerism: hydration isomers

- Hydration isomers result from the interchange of  $\text{H}_2\text{O}$  and another ligand between the first coordination sphere and the ligands outside it.
  - $\text{CrCl}_3 \cdot 6\text{H}_2\text{O}$ , actually  $[\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2]\text{Cl} \cdot 2\text{H}_2\text{O}$
  - When this is dissolved in water, the chloride ions in the complex are slowly replaced by water to give blue-green  $[\text{Cr}(\text{H}_2\text{O})_5\text{Cl}]\text{Cl}_2 \cdot \text{H}_2\text{O}$  and finally violet  $[\text{Cr}(\text{H}_2\text{O})_6]\text{Cl}_3$

# Structural isomerism: coordination isomerism

- Coordination isomers are possible only for **salts in which both cation and anion are complex ions**; the isomers arise from interchange of ligands between the two metal centres.

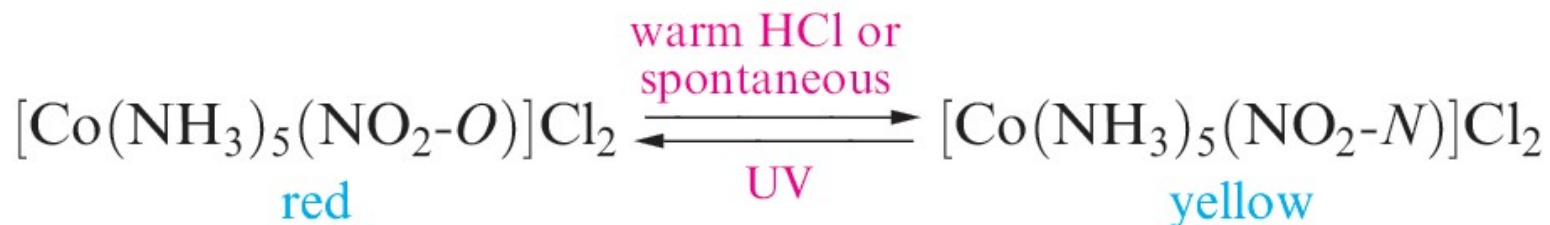
Examples of coordination isomers are:

- $[\text{Co}(\text{NH}_3)_6][\text{Cr}(\text{CN})_6]$  and  $[\text{Cr}(\text{NH}_3)_6][\text{Co}(\text{CN})_6]$ ;
- $[\text{Co}(\text{NH}_3)_6][\text{Co}(\text{NO}_2)_6]$  and  $[\text{Co}(\text{NH}_3)_4(\text{NO}_2)_2][\text{Co}(\text{NH}_3)_2(\text{NO}_2)_4]$ ;
- $[\text{Pt}^{\text{II}}(\text{NH}_3)_4][\text{Pt}^{\text{IV}}\text{Cl}_6]$  and  $[\text{Pt}^{\text{IV}}(\text{NH}_3)_4\text{Cl}_2][\text{Pt}^{\text{II}}\text{Cl}_4]$ .

# Structural isomerism: linkage isomerism

- Linkage isomers may arise when one or more of the ligands can coordinate to the metal ion in more than one way.

– linkage isomers of  $[\text{Co}(\text{NH}_3)_5(\text{NO}_2)]^{2+}$



- distinguished by using IR spectroscopy.
  - For the O-bonded ligand, characteristic absorption bands at 1065 and 1470  $\text{cm}^{-1}$
  - while for the N-bonded ligand, the corresponding vibrational wavenumbers are 1310 and 1430  $\text{cm}^{-1}$ .

# Structural isomerism: polymerization isomerism

- Polymerization isomers denote complexes which have the same empirical formulae but different molecular masses.

Examples of polymerization isomers are:

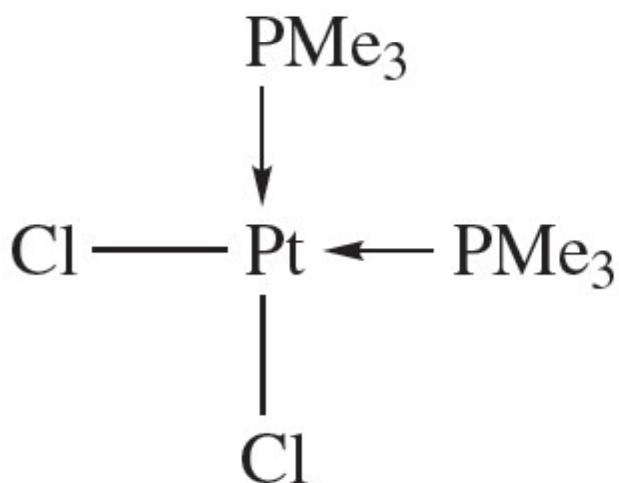
- $[\text{PtCl}_2(\text{NH}_3)_2]$  and  $[\text{Pt}(\text{NH}_3)_4][\text{PtCl}_4]$ ;
- $[\text{Co}(\text{NH}_3)_3(\text{NO}_2)_3]$  and  $[\text{Co}(\text{NH}_3)_6][\text{Co}(\text{NO}_2)_6]$ .

# Stereoisomerism: geometrical isomers

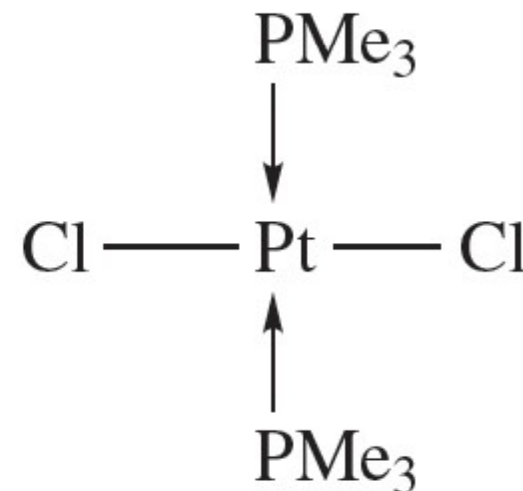
- If two species have the same molecular formulae and the same structural framework, but **differ in the spatial arrangement** of different atoms or groups about a central atom or a double bond, then the compounds are geometrical isomers.
- **Square planar** , **Octahedral** and **Trigonal Bipyramidal** species

# Stereoisomerism: geometrical isomers

- Square planar species:
  - Square planar species of the general form  $\text{EX}_2\text{Y}_2$  or  $\text{EX}_2\text{YZ}$  may possess cis- and trans-isomers.



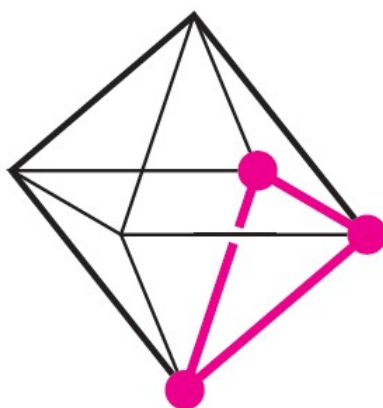
*cis-isomer*



*trans-isomer*

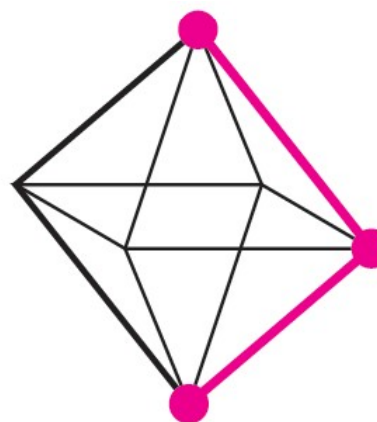
# Stereoisomerism: geometrical isomers

- Octahedral species:
  - An octahedral species containing three identical groups (e.g. of type  $\text{EX}_3\text{Y}_3$ ) may possess *fac*- and *mer*-isomers..



*Facial*  
arrangement

*fac*-isomer

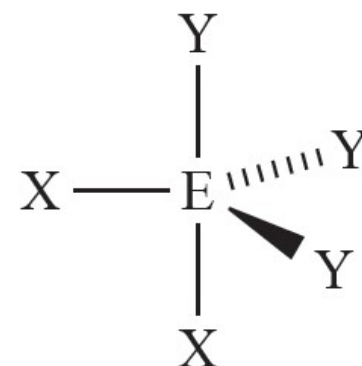
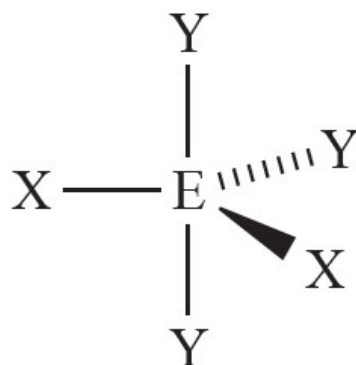
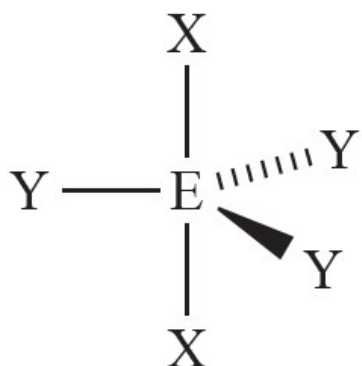


*Meridional*  
arrangement

*mer*-isomer

# Stereoisomerism: geometrical isomers

- Trigonal bipyramidal species:
  - In a trigonal bipyramidal species, geometrical isomerism arises because of the presence of axial and equatorial sites.



Steric factors may dictate which isomer is preferred for a given species

e.g. static structure of  $\text{PCl}_3\text{F}_2$ .

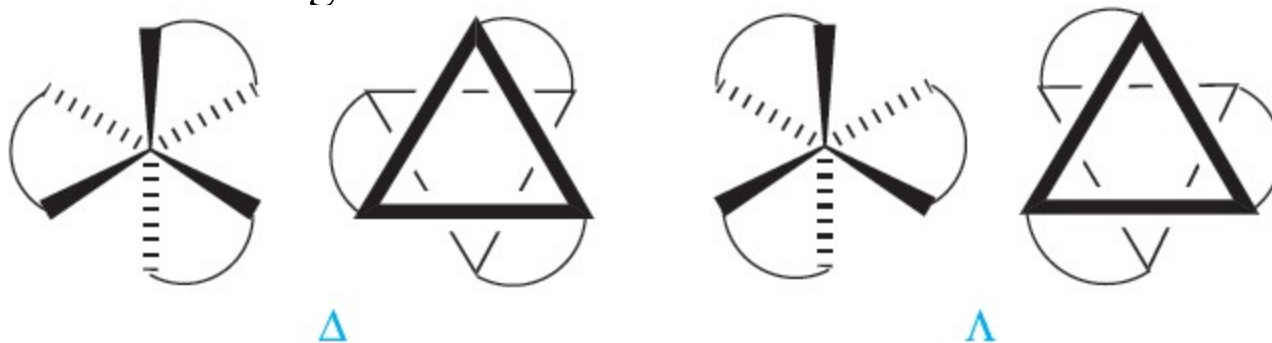


# Stereoisomerism: optical isomers

- Optical isomerism is concerned with chirality, and some important terms relating to chiral complexes
- **Enantiomers** are a pair of stereoisomers that are nonsuperposable mirror images
- (+) and (-) prefixes
  - specific rotation
  - Sign of  $[\alpha]_D$ .
- *d* and *l* prefixes :
  - dextro- and laevo- (derived from the Latin for right and left)
  - refer to right- and left-handed rotation of the plane of polarized light respectively
- The +/- or *d/l* notation is not a direct descriptor of the absolute configuration of an enantiomer (the arrangement of the substituents or ligands) for which the following
- prefixes are used.

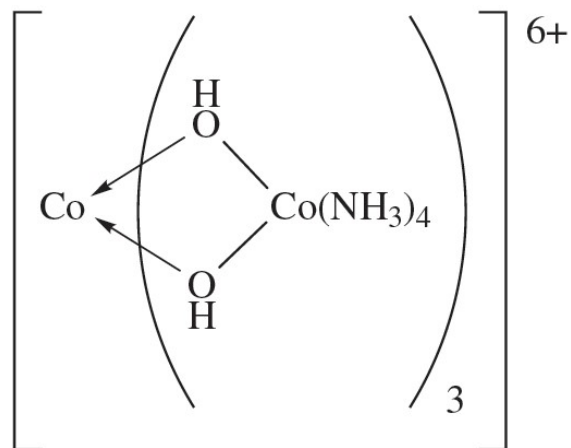
# Stereoisomerism: optical isomers

- *R* and *S* prefixes: Cahn–Ingold–Prelog notation
  - notation is used for chiral organic ligands, and also for tetrahedral complexes
  - The *R*- and *S*-labels for the enantiomers refer to a clockwise (rectus) and anticlockwise (sinister) sequence of the prioritized atoms, working from high to low.
- $\Delta$  and  $\Lambda$  prefixes:
  - enantiomers of octahedral complexes containing three equivalent didentate ligands (tris-chelate complexes)
  - octahedron is viewed down a three-fold axis, and the chelates then define either a right- or left-handed helix.

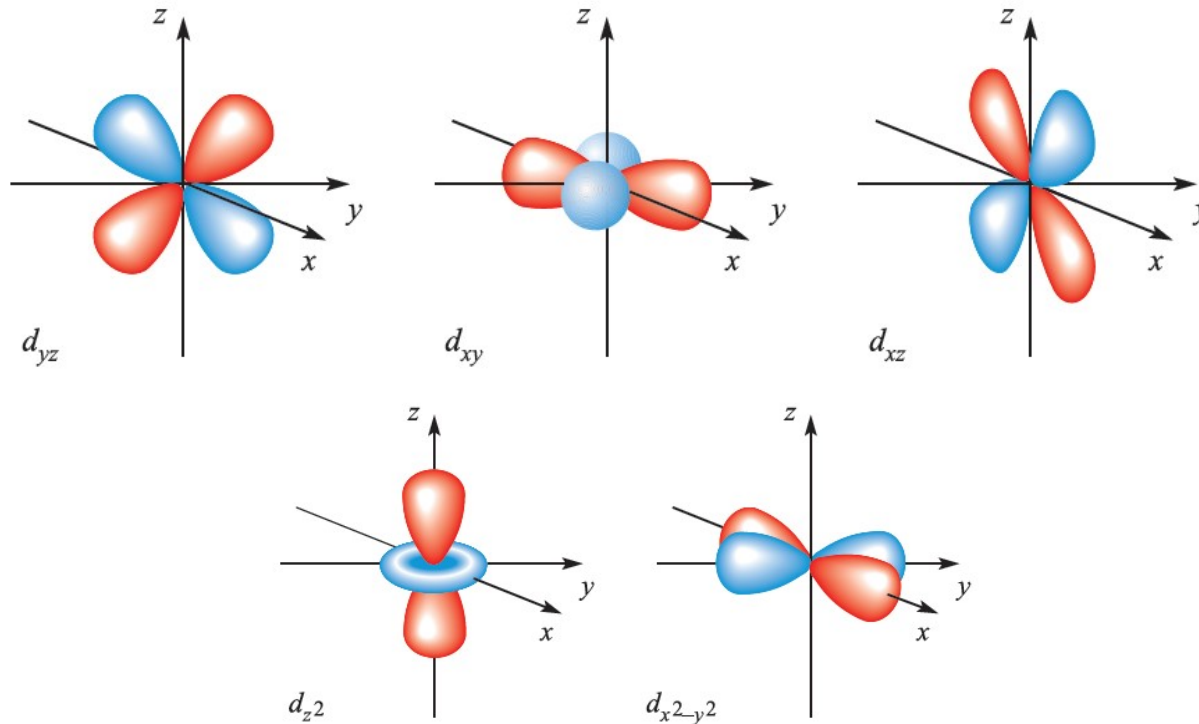


# Stereoisomerism: optical isomers

- Bis-chelate octahedral complexes : cis- and trans-isomers
  - $[\text{Co}(\text{en})_2\text{Cl}_2]^+$
- The first purely inorganic complex to be resolved into its optical isomers was



# Spatial orientation of d-orbitals



**consequence of this difference:** the d orbitals in the presence of ligands are **split into groups of different energies**, the type of splitting and the magnitude of the energy differences depending on the **arrangement and nature of the ligands**.

The ‘mixing’ or ‘blending’ of atomic orbitals to accommodate the spatial requirements in a molecule is known as *hybridization*.

Hybridization occurs to minimize electron pair repulsions when atoms are brought together to form molecules.

2 <sup>nd</sup> row elements:	$sp$	$sp^2$	$sp^3$
3 <sup>rd</sup> row elements also have:		$dsp^3$	$d^2sp^3$

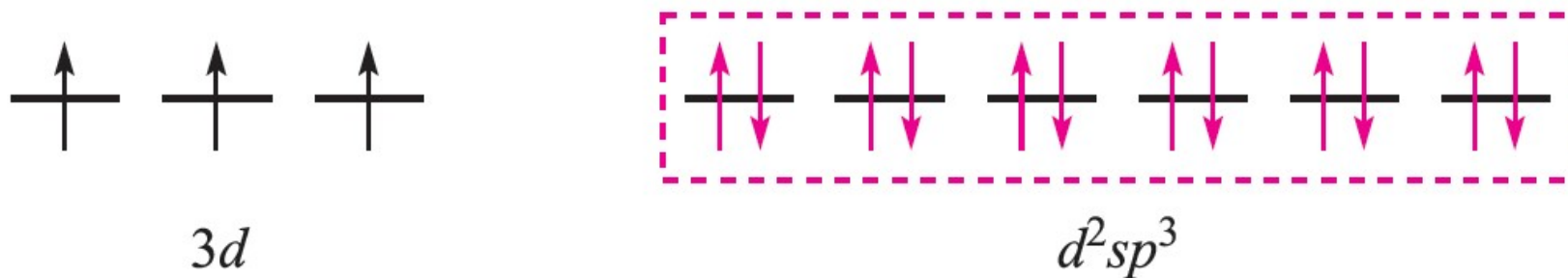
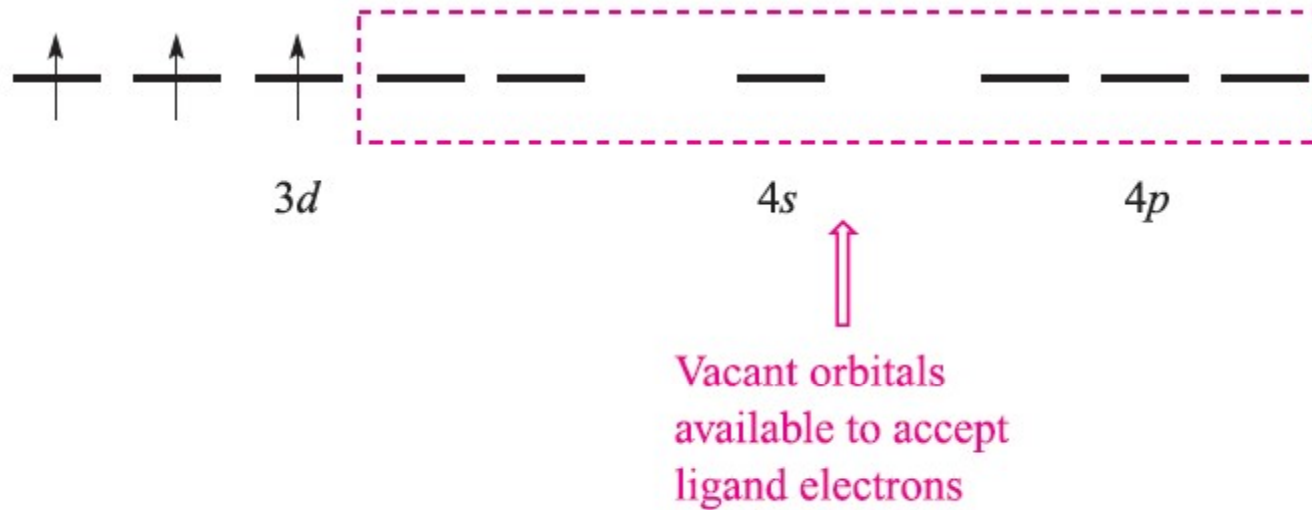
Bonding arises from the overlap of orbitals.

Sigma ( $\sigma$ ) bonds arise from the ‘end-on’ overlap between adjacent orbitals. This leads to a region of high electron density along the inter-nuclear axis (cylindrically symmetrical).

# valence bond theory

Coordination number	Arrangement of donor atoms	Orbitals hybridized	Hybrid orbital description	Example
2	Linear	$s, p_z$	$sp$	$[\text{Ag}(\text{NH}_3)_2]^+$
3	Trigonal planar	$s, p_x, p_y$	$sp^2$	$[\text{HgI}_3]^-$
4	Tetrahedral	$s, p_x, p_y, p_z$	$sp^3$	$[\text{FeBr}_4]^{2-}$
4	Square planar	$s, p_x, p_y, d_{x^2-y^2}$	$sp^2d$	$[\text{Ni}(\text{CN})_4]^{2-}$
5	Trigonal bipyramidal	$s, p_x, p_y, p_z, d_{z^2}$	$sp^3d$	$[\text{CuCl}_5]^{3-}$
5	Square-based pyramidal	$s, p_x, p_y, p_z, d_{x^2-y^2}$	$sp^3d$	$[\text{Ni}(\text{CN})_5]^{3-}$
6	Octahedral	$s, p_x, p_y, p_z, d_{z^2}, d_{x^2-y^2}$	$sp^3d^2$	$[\text{Co}(\text{NH}_3)_6]^{3+}$
6	Trigonal prismatic	$s, d_{xy}, d_{yz}, d_{xz}, d_{z^2}, d_{x^2-y^2}$ or $s, p_x, p_y, p_z, d_{xz}, d_{yz}$	$sd^5$ or $sp^3d^2$	$[\text{ZrMe}_6]^{2-}$
7	Pentagonal bipyramidal	$s, p_x, p_y, p_z, d_{xy}, d_{x^2-y^2}, d_{z^2}$	$sp^3d^3$	$[\text{V}(\text{CN})_7]^{4-}$
7	Monocapped trigonal prismatic	$s, p_x, p_y, p_z, d_{xy}, d_{xz}, d_{z^2}$	$sp^3d^3$	$[\text{NbF}_7]^{2-}$
8	Cubic	$s, p_x, p_y, p_z, d_{xy}, d_{xz}, d_{yz}, f_{xyz}$	$sp^3d^3f$	$[\text{PaF}_8]^{3-}$
8	Dodecahedral	$s, p_x, p_y, p_z, d_{z^2}, d_{xy}, d_{xz}, d_{yz}$	$sp^3d^4$	$[\text{Mo}(\text{CN})_8]^{4-}$
8	Square antiprismatic	$s, p_x, p_y, p_z, d_{xy}, d_{xz}, d_{yz}, d_{x^2-y^2}$	$sp^3d^4$	$[\text{TaF}_8]^{3-}$
9	Tricapped trigonal prismatic	$s, p_x, p_y, p_z, d_{xy}, d_{xz}, d_{yz}, d_{z^2}, d_{x^2-y^2}$	$sp^3d^5$	$[\text{ReH}_9]^{2-}$

# Chromium (III): Octahedral

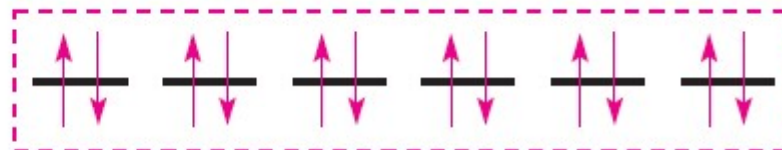




# Fe<sup>3+</sup> ion: Octahedral



*3d*

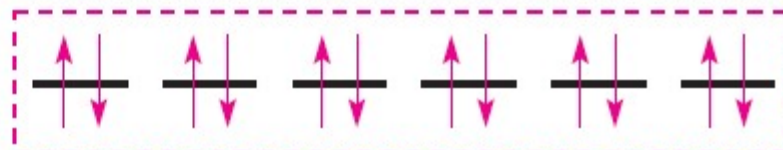


*d<sup>2</sup>sp<sup>3</sup>*

Low spin: paramagnetic



*3d*



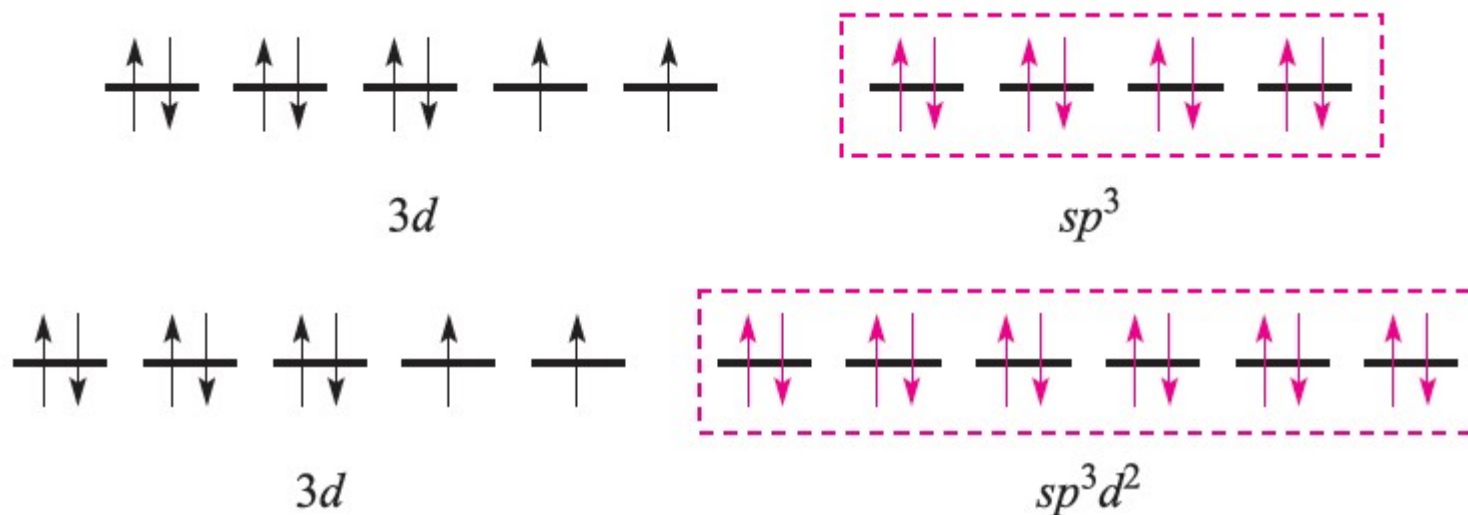
*sp<sup>3</sup>d<sup>2</sup>*

High spin, but **unrealistic**: paramagnetic



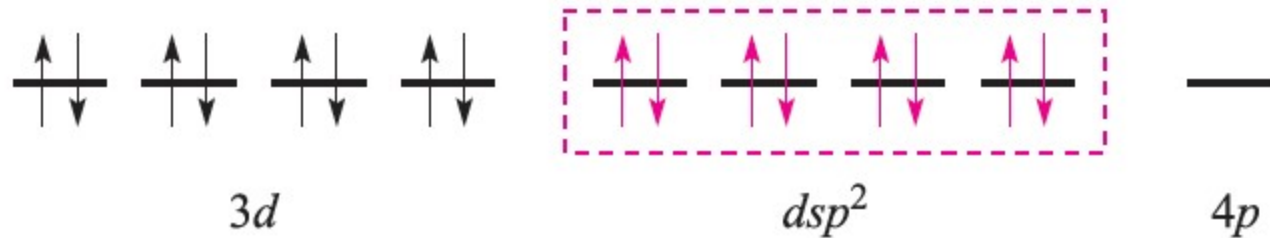
# Ni<sup>2+</sup> ion: Octahedral vs Tetrahedral

- Nickel(II) (d<sup>8</sup>) forms **paramagnetic tetrahedral and octahedral complexes**.



## Ni<sup>2+</sup> ion: Square Planar

- Nickel(II) ( $d^8$ ) forms **diamagnetic square planar complexes.**



# Limitations

- It can say nothing about **electronic spectroscopic properties** .
- **Chemical reactivity** can't be predicted
  - kinetic inertness that is a characteristic of the low-spin d 6 configuration.
- Furthermore, the model implies a **distinction between high- and low-spin complexes** that is actually **misleading**.
- Finally, it cannot tell us why certain ligands are associated with the **formation of high- (or low-)spin complexes**.