

## 17: Introduction to Coordination Chemistry

### Key Inorganic Terms

**Coordination compound or Coordination complex** is a compound between a metal and attached ligands. These complexes can be neutral or ionic, with the appropriate counterions.

**Coordination number** is the number of ligands directly attached to the metal.

**Ligands** are ions or small molecules that are bonded to a metal, often through coordinate covalent bonds. Some common ligands are halides, CO, water, ammonia, aromatic compounds or ions, and many other small molecules.

**A Werner complex** is a coordination compound consisting of a metal and ligands.

**Isomers** are different compounds with the same molecular formula.

**Constitutional isomers** are isomers in which the atoms are connected differently. Special cases are Hydrate, Ionization, Coordination, and Linkage isomers.

**Stereoisomers** are isomers with the same atom connectivity but different orientation of the atoms in space.

**Enantiomers** are stereoisomers that are non-superimposable (not identical) mirror images of each other. **Diastereomers** are stereoisomers that are not enantiomers. Cis and trans isomers are examples of diastereomers.

**A chiral compound** is one that is not superimposable on its mirror image. Chiral compounds are optically active. This means that they rotate polarized light in one direction. A **racemic mixture** is a mixture of both enantiomers of a chiral compound. A racemic mixture is not optically active, but each of the enantiomers separately are optically active.

**A chelate** is a complex in which one or more ligands are attached to the metal via more than one atom. Ligands that attach to the metal at 2 or more points are called **chelating ligands**.

**The octet rule** says that stable molecules have an octet (8) of valence electrons. For hydrogen, an "octet" is 2 electrons. There are many exceptions to the octet rule.

**The 18 electron rule** is an extension of the octet rule to transition metal compounds. As with the octet rule, there are many exceptions. Stable 16 electron complexes are particularly common.

**Degenerate orbitals** are orbitals that have the same energy. Degeneracy is a consequence of symmetry.

**Crystal field theory** is a simple electrostatic model that explains the structure of transition metal complexes. The negative charge from the ligand lone pairs breaks the degeneracy of the 5 d-orbitals, raising the energy of the orbitals nearest the incoming ligands. This results in the familiar orbital energy splitting in 4 and 6 coordinate complexes.

**Ligand field theory** is an approximate molecular orbital treatment of the metal-ligand bonding in transition metal complexes.

### Common Coordination Numbers

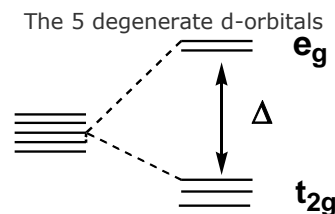
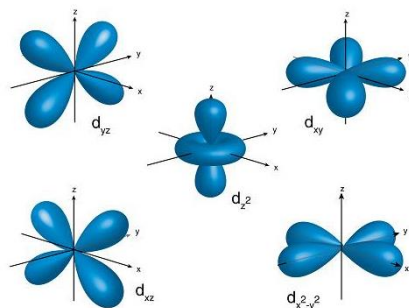
**CN 4** may be a tetrahedral or square planar geometry.

**CN 5** may be a trigonal bipyramid or square pyramid structure. More often, it is intermediate between those geometries, or a fluxional structure in which the geometries rapidly interchange.

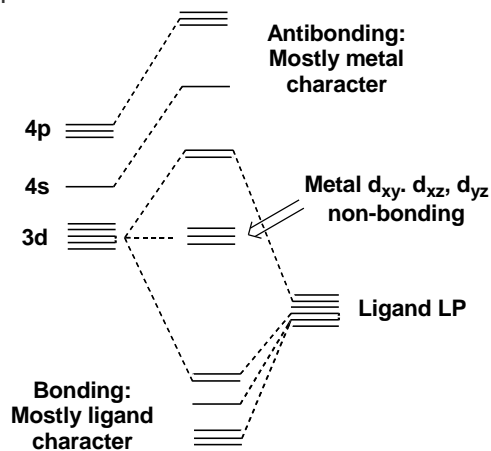
**CN 6** is usually an octahedral structure, but trigonal prism geometries are also known. There are some rare cases of other 6-coordinate geometries.

**CN 7** may take on several geometries or an intermediate structure. Coordination numbers of higher than 7 are found mostly in heavy metal complexes, with large metal atoms and small ligands. One example is  $\text{ReH}_9$ .

### Illustration of Crystal Field and Ligand Field Theory in Octahedral Complexes.



As the 6 ligands approach the metal, the orbitals along the Cartesian axes are raised in energy relative to those between the axes.



Ligand field theory describes the interaction between the metal and the ligand orbitals. In an octahedral complex, the  $d_{xy}$ ,  $d_{xz}$ , and  $d_{yz}$  orbitals remain non-bonding.

How to Use This Cheat Sheet: These are the keys related this topic. Try to read through it carefully twice then recite it out on a blank sheet of paper. Review it again before the exams.