Coordination Compounds:

“Gedanken” experiment: CuCl$_2$ blue crystals → dissolve in water to pale blue solution → start adding HCl solution until it turns yellow → start bubble through NH$_3$ and color changes to green and than deep blue

What's happening? ⇒ intense competition of H$_2$O, Cl$^-$, NH$_3$ for Cu$^{2+}$ and H$^+$ ions (acid/base chemistry)

Electronic and geometric structures explain the stability, optical and magnetic properties.

Naming of Coordination Compounds:

1. determine the oxidation state of the metal
2. name the ligands and order them alphabetically
3. add the names of the counter-ions without specifying their number
4. do not use twice the same numerical prefix for the same ligand (no di____di____, rather bis____di____)

Geometric Structures:

- coordination number: 3-12, most frequent C.N.-s are 4-6 (tetra-, penta-, and hexacoordinate)
- coordination geometry:
  - C.N. = 6 ⇒ octahedral, tetragonal bipyramidal, trigonal prismatic
  - C.N. = 5 ⇒ trigonal bipyramidal, tetragonal pyramidal
  - C.N. = 4 ⇒ tetrahedral, tetragonal planar

Electronic Structures:

- **Valence bond model:** (uses the valence electrons and operates with hybridizations)
  - $d^3sp^3 \rightarrow (z, z^2) \ (s,x^2-y^2) \ (s,y,x^2-y^2)$ typical for $d^6$ metals + 6 2e$^-$ donor ligands
  - $dsp^3 \rightarrow (s,x,x^2-y^2) \ (s,y,x^2-y^2)$ typical for $d^8$ metals + 4 2e$^-$ donor ligands

- **Crystal field theory:** (determines the electron repulsion among the d- and the ligand electrons)
  - Fe$^{3+}$ ion in gas phase → the d manifold is degenerate
  - FeCl$_3$ in aqueous solution → [Fe$^{3+}$OH$_3$]Cl$_3$ → octahedral coordination ⇒ d orbitals split
    - a) set of d-orbitals close to the ligand electrons: $z^2$, $x^2-y^2$ – Group Theory: $e_g$
    - b) set of d-orbitals away from the ligand electrons: $xy$, $xz$, $yz$ – Group Theory: $t_{2g}$
  - (Et$_4$N)$_2$[Ni(SEt)$_4$] in organic solution (ACN or DMF) remains tetrahedral ⇒ d orbitals split
    - a) set of d-orbitals close to the ligand electrons: $xy$, $xz$, $yz$ – Group Theory: $t_2$
    - b) set of d-orbitals away from the ligand electrons: $z^2$, $x^2-y^2$ – Group Theory: $e$

- magnitude of the splitting is determined by the number and nature of the ligands (spectrochemical series), charge and size of the metal
  - strong-field ligands ⇒ induce large splitting ⇒ resulting in low spin complexes
  - weak-field ligands ⇒ induce small splitting ⇒ results in high spin complexes

- spectroscopy: the magnitude of d-orbital splitting is in the range of UV/VIS light (400-700 nm) ⇒ various excitations of lower lying d-electrons to higher lying empty d-orbitals by absorbing light gives the color of coordination compounds