



CHELATES & CHELATING AGENTS

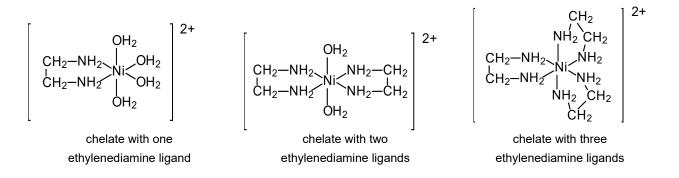
Many essential biological chemicals are chelates. Chelates play important roles in oxygen transport and in photosynthesis. Furthermore, many biological catalysts (enzymes) are chelates. In addition to their significance in living organisms, chelates are also economically important, both as products in themselves and as agents in the production of other chemicals.

A chelate is a chemical compound composed of a metal ion and a chelating agent. A chelating agent is a substance whose molecules can form several bonds to a single metal ion. In other words, a chelating agent is a multidentate ligand. An example of a simple chelating agent is ethylenediamine.

NH2-CH2-CH2-NH2

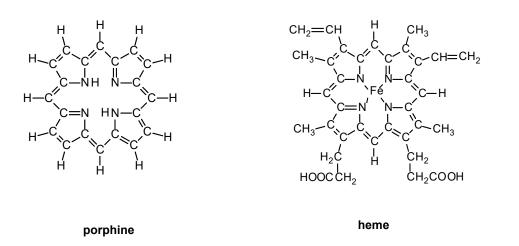
ethylenediamine

A single molecule of ethylenediamine can form two bonds to a transition-metal ion such as nickel(II), Ni^{2+} . The bonds form between the metal ion and the nitrogen atoms of ethylenediamine. The nickel(II) ion can form six such bonds, so a maximum of three ethylenediamine molecules can be attached to one Ni^{2+} ion.



In the two structures on the left, the bonding capacity of the Ni^{2+} ion is completed by water molecules. Each water molecule forms only one bond to Ni^{2+} , so water is not a chelating agent. Because the chelating agent is attached to the metal ion by several bonds, chelates tend to be more stable than complexes formed with monodentate ligands such as water.

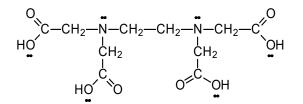




Porphine is a chelating agent similar to ethylenediamine in that it forms bonds to a metal ion through nitrogen atoms. Each of the four nitrogen atoms in the center of the molecule can form a bond to a metal ion. Porphine is the simplest of a group of chelating agents called porphyrins. Porphyrins have a structure derived from porphine by replacing some of the hydrogen atoms around the outside with other groups of atoms. One important porphyrin chelate is heme, the central component of hemoglobin, which carries oxygen through the blood from the lungs to the tissues. Heme contains a porphyrin chelating agent bonded to an iron(II) ion. Iron, like nickel, can form six bonds. Four of these bonds tie it to the porphyrin. One of iron's two remaining bonds holds an oxygen molecule as it is transported through the blood. Chlorophyll is another porphyrin chelate. In chlorophyll, the metal at the center of the chelate is a magnesium ion. Chlorophyll, which is responsible for the green color of plant leaves, absorbs the light energy that is converted to chemical energy in the process of photosynthesis.

Another biologically significant chelate is vitamin B-12. It is the only vitamin that contains a metal, a cobalt(II) ion bonded to a porphyrin-like chelating agent. As far as is known, it is required in the diet of all higher animals. It is not synthesized by either higher plants or animals, but only by certain bacteria and molds. These are the sources of the B-12 found in animal products. Because vitamin B-12 is not found in higher plants, vegetarians must take care to include in their diets foods or supplements that contain the vitamin.

A chelating agent of particular economic significance is ethylenediaminetetraacetic acid (EDTA).



ethylenediaminetetraacetic acid (EDTA)

EDTA is a versatile chelating agent. It can form four or six bonds with a metal ion, and it forms chelates with both transition-metal ions and main-group ions. EDTA is frequently used in soaps and detergents, because it forms a complexes with calcium and magnesium ions. These ions are in hard water and interfere with the cleaning action of soaps and detergents. The EDTA binds to them, sequestering them and preventing their interference. In the calcium complex, $[Ca(EDTA)]^{2-}$, EDTA is a tetradentate ligand, and chelation involves the two nitrogen atoms and two oxygen atoms in separate carboxyl (-COO⁻) groups. EDTA is also used extensively as a stabilizing agent in the food industry. Food spoilage is often promoted by naturally-occurring enzymes that contain transition-metal ions. These enzymes catalyze the chemical reactions that occur during spoilage. EDTA deactivates these enzymes by removing the metal ions from them and forming stable chelates with them. It promotes color retention in dried bananas, beans, chick peas, canned clams, pecan pie filling, frozen potatoes, and canned shrimp. It improves flavor retention in canned carbonated beverages, salad dressings, mayonnaise, margarine, and sauces. It inhibits rancidity in salad dressings, mayonnaise, sauces, and sandwich spreads. EDTA salts are used in foods at levels ranging from 33 to 800 ppm.

In other applications, EDTA dissolves the CaCO₃ scale deposited from hard water without the use of corrosive acid. EDTA is used in the separation of the rare earth elements from each other. The rare earth elements have very similar chemical properties, but the stability of their EDTA complexes varies slightly. This slight variation allows EDTA to effectively separate rare-earth ions. EDTA is used as an anticoagulant for stored blood in blood banks; it prevents coagulation by sequestering the calcium ions required for clotting. As an antidote for lead poisoning, calcium disodium EDTA exchanges its chelated calcium for lead, and the resulting lead chelate is rapidly excreted in the urine. The calcium salt of EDTA, administered intravenously, is also used in the treatment of acute cadmium and iron poisoning.

Dimercaprol (2,3-dimercapto-1-propanol) is an effective chelating agent for heavy metals such as arsenic, mercury, antimony, and gold. These heavy metals form particularly strong bonds to the sulfur atoms in dimercaprol.

SH

$$HO-CH_2-CH-CH_2-SH + Hg^2 + \longrightarrow HO-CH_2-CH-S$$

dimercaprol
 $HO-CH_2-CH-CH_2-SH + Hg^2 + \longrightarrow HO-CH_2-CH-S$

Dimercaprol was originally employed to treat the toxic effects of an arsenic-containing mustard gas called Lewisite [dichloro(2-chlorovinyl)arsine], which was used in World War I. The chelated metal cannot enter living cells and is rapidly excreted from the body. Since dimercaprol is water insoluble, it is dissolved in an oil base (often peanut oil) and injected intramuscularly.