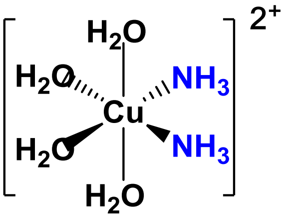
Newcastle University

# The Chelate Effect

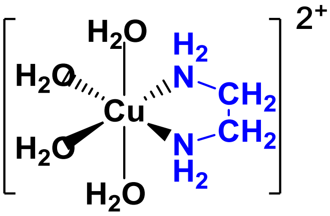
The Chelate Effect (from Greek *chele*, meaning 'claw') occurs when simple, unidentate ligands (such as $H_2O$ or $NH_3$) are replaced by bidentate or multidentate ligands such as 1,2-diaminoethane (en) or EDTA in a metal complex. This makes the complex far more stable, since it is more difficult to break a larger number of bonds at the same time.

**For example:**



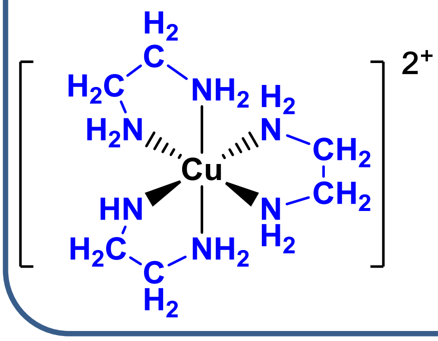

**$[Cu(NH_3)_2(H_2O)_4]^{2+}$** (6 x unidentate ligands)

Stability constant of complex (log K) = **7.9**




**$[Cu(H_2O)_4(en)]^{2+}$** (4 x unidentate ligands, 1 x bidentate ligand)

Stability constant of complex (log K) = **10.6**

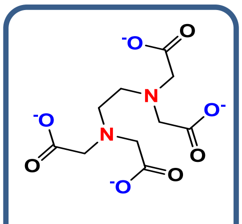



The en ligand is far more stable than 2 unidentate ligands. The complexes above could easily react further to produce the complex **$[Cu(en)_3]^{2+}$**. This complex has a stability constant of 18.7.

**TOP TIP!**
The higher the stability constant, the more stable the complex. This means it's less reactive!


# EDTA – as stable as it gets

EDTA is a multidentate ligand, which is able to attach to the central metal by **up to** six atoms (4 oxygen and 2 nitrogen atoms). EDTA has an overall 4- charge.



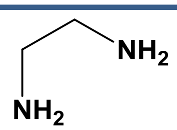

$EDTA^{4-}$

## Enthalpy:

You might think that enthalpy changes could affect complex stabilities. This is not the case. When looking carefully, you are only actually breaking and making bonds around the central metal. In each case, you break and make the similar (or the same) bonds. This is irrespective of what ligands are attached to the central metal.

**For example:**

$$[Cu(H_2O)_6]^{2+} + 2NH_3 \rightleftharpoons [Cu(NH_3)_2(H_2O)_4]^{2+} + 2H_2O$$
$$[Cu(H_2O)_6]^{2+} + en \rightleftharpoons [Cu(en)(H_2O)_4]^{2+} + 2H_2O$$



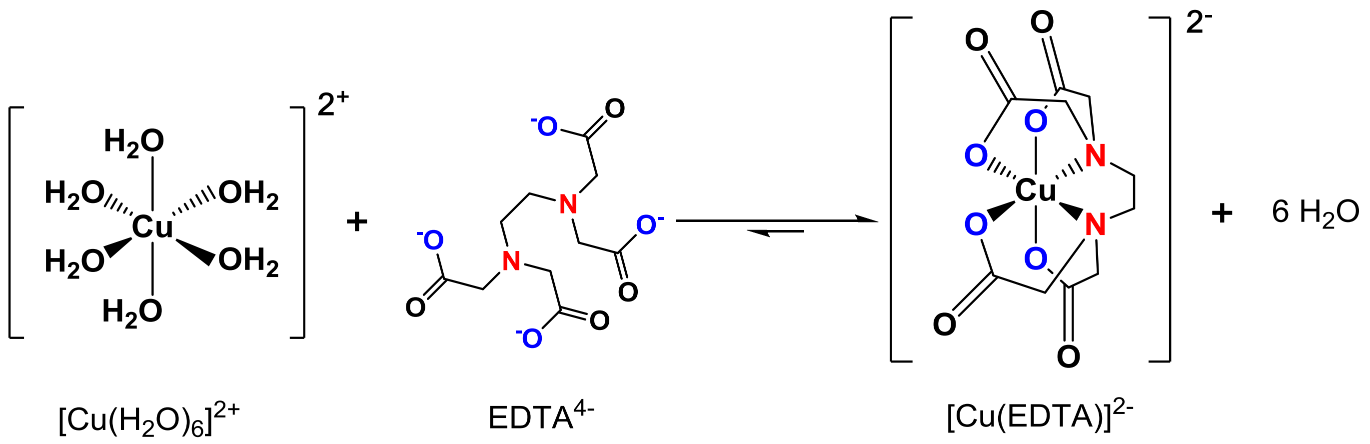

Ethylenediamine (en)

In both reactions, you break two C-O bonds and make two C-N bonds. The reaction enthalpies are therefore very similar. Enthalpy is therefore not the reason.

## Entropy:

As you should already know, entropy is the **measure of disorder**. An increase of disorder is preferable in a reaction. This means that if there is positive entropy (an increasing number of moles/molecules etc), the reaction is more likely to occur.

Take the reaction between $[Cu(H_2O)_6]^{2+}$ and $EDTA^{4-}$ for example:




In this reaction, there are only two species (1 x copper complex, 1 x EDTA ligand) on the reactants side. On the side of the products, there are seven species (1 x copper complex, 6 x $H_2O$ molecules).

This means that there is a major **increase in disorder** from the **reactants** to the **products**. It is very difficult to move from a lot of disorder to little disorder. This is why the EDTA complex is so stable.

$$\Delta G = \Delta H - T\Delta S$$

When considering a reaction, remember that the Gibbs' free energy ($\Delta G$) must **always** be $\leq 0$ for a reaction to occur spontaneously. This means that the $T\Delta S$ function must be greater than the $\Delta H$ function. This is why reactions generally occur more spontaneously at higher temperatures.

When adding a **multidentate** EDTA ligand to $[Cu(H_2O)_6]^{2+}$, the $\Delta G$ value is far lower than when the unidentate water ligands are replaced with other **unidentate** ligands. For this reason, a $[M(EDTA)]^{n-}$ complex is **almost** impossible to break down.

**The 'equilibrium' above is therefore not really an equilibrium reaction at all.**