Chem Factsheet

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EDTA - (Ethylenediaminetetraacetic acid)

To succeed in this topic you will need to:
- understand the concept of coordinate bonding (Factsheets 05 and 179)
- understand the concept of complex formation and ligand substitution in transition metal ions (Factsheet 46)
- understand the concept of entropy (Factsheet 194)

After working through this Factsheet you will be able to:
- draw the structure of EDTA
- explain why EDTA can act as a hexadentate ligand
- describe how EDTA forms complexes in terms of coordinate bonding to a central metal ion
- understand the relative stability of EDTA complexes
- describe the chelating effect of EDTA
- give the common uses of EDTA

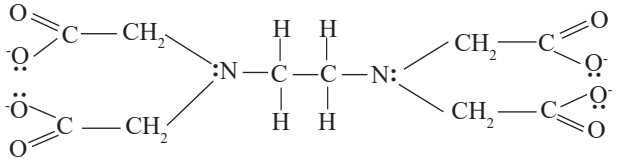
Structure of EDTA

Ethylenediaminetetraacetic acid (EDTA) is a colourless, water-soluble solid with the molecular formula $C_{10}H_{16}N_2O_8$ and a molar mass of 292 $gmol^{-1}$

The molecule is essentially ethane-1,2-diamine with each of the hydrogen atoms on the nitrogen atoms substituted by $–CH_2COOH$ groups - hence "tetraacetic acid" since acetic acid is the old name for ethanoic acid, CH_3COOH.

When dissolved in water, the four hydrogens of the –OH groups dissociate to form the conjugate base ethylenediaminetetraacetate, $EDTA^{4-}$.

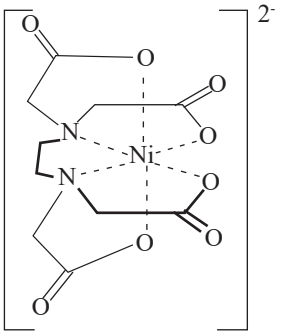
Fig. 1 $EDTA^{4-}$ showing lone pairs of electrons



Formation of Complexes

$EDTA^{4-}$ forms six coordinate (dative) bonds to a central metal ion (e.g. Ni^{2+}) due to the lone pairs of electrons identified in figure 1. It is therefore described as a multidentate, or more specifically a hexadentate, ligand. The angle of the bonds around the central metal ion is 90° so therefore it forms an octahedral shape as shown in Fig. 2.

Fig. 2 $[NiEDTA]^{2-}$ complex



$EDTA^{4-}$ will substitute other monodentate and bidentate ligands around central metal ions. In the equation below, the six water ligands surrounding the Co^{2+} ion are substituted by one $EDTA^{4-}$ molecule.

$$[Co(H_2O)_6]^{2+}(aq) + EDTA^{4-}(aq) \rightleftharpoons [Co(EDTA)]^{2-}(aq) + 6H_2O(l)$$

The reaction has a significantly positive entropy change (ΔS : remember: entropy is a measure of disorder) since seven product particles are formed from two reactant particles.

Also, ΔH for the reaction is approximately zero because six coordinate bonds are replaced by six similar coordinate bonds.

Thus ΔG (Gibbs' Free Energy change) for this reaction will always be negative since $\Delta G = \Delta H - T\Delta S$

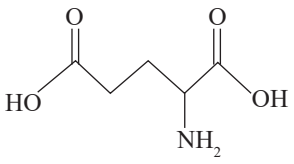
Consequently, complexes containing $EDTA^{4-}$ are generally more stable than those containing mono- and bidentate ligands.

This means that generally any metal ion in a complex with mono- and bidentate ligands will react with $EDTA^{4-}$ and these ligands will be substituted.

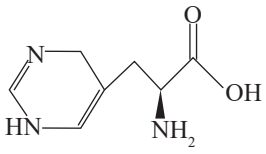
The Chelating Effect

The ability of $EDTA^{4-}$ to substitute other ligands is called the chelating effect and so $EDTA^{4-}$ is described as a chelating agent. A chelating agent has a greater affinity for a metal ion than non-chelating ligands e.g. monodentate ligands.

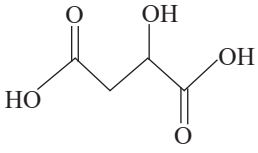
Many natural chelating agents exist, including the amino acids glutamic acid and histidine and organic dicarboxylic acid salts such as malate derived from malic acid.



Glutamic acid

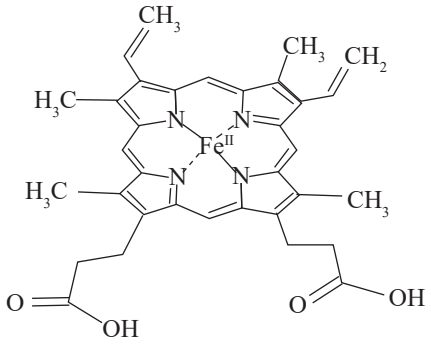


Histidine

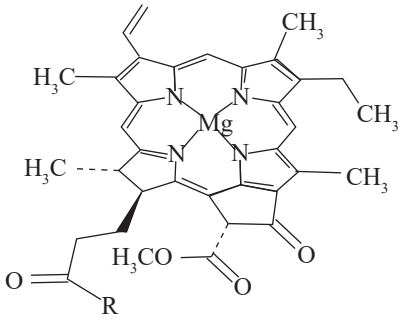


Malic acid

The Fe^{2+} ion in haemoglobin and the Mg^{2+} ion in chlorophyll are chelated by the porphyrin rings that form the co-factors of the proteins.



Chelation in haemoglobin



Chelation in chlorophyll

EDTA is a synthetic chelating agent and was first described in 1935. Today, about 80,000 tonnes of EDTA are produced each year. Its wide-ranging uses are dependent on its strong chelating abilities. It sequesters (isolates or hides) metal ions. Once bound to EDTA, the reactivity of the metal ions is significantly diminished.

Questions

1. Draw the skeletal formula of EDTA.
2. Write a balanced equation for the reaction of EDTA with sodium hydroxide.
3. Suggest how the structure of EDTA will change in the presence of a strong acid.
4. Write an equation to show the chelation of aqueous Cu^{2+} ions by $EDTA^{4-}$.
5. Explain why complexes containing $EDTA^{4-}$ are more stable than those containing monodentate ligands.

Uses of EDTA

Since $EDTA^{4-}$ will sequester metal ions and therefore diminish their reactivity, it is often used in situations where metal ions need to be removed from a system. A few examples of the wide-ranging uses of EDTA are considered on this Factsheet.

Lead Poisoning Treatment

Lead is toxic to many organs of the body and is a potent neurotoxin with the potential to cause serious damage to the nervous system. It is particularly dangerous to the developing brain and can result in serious learning and behavioural disorders.

Contaminated water and consumer products (including lead-based paints) are the most common means of exposure to lead. Lead-based paint was banned from sale in the UK in 1992 and is now only available for specialist uses. Lead compounds were included in paint as the main white pigment.

EDTA in the form of disodium calcium EDTA ($CaNa_2EDTA$) is used in a procedure called chelation therapy. The EDTA sequesters the lead ions forming a non-toxic complex which is then excreted in the urine. Side-effects can result from this treatment since EDTA will also sequester necessary nutrients such as zinc.

It is also used to treat cases of thalassemia caused by overload of iron in the body.

Blood Analysis

A full blood count (FBC) is a widely used blood test in which the number of each of the different types of blood cells in a sample of blood is measured. It gives an indication about possible health problems including anaemia, lung disease and viral and bacterial infections.

The blood is often taken and drawn into a tube containing EDTA which acts as an anticoagulant, i.e. it stops it from clotting so that the cells can be counted. The EDTA binds and deactivates calcium ions which are an essential component in the activation of the clotting factors in the blood.

Reducing Water Hardness

The presence of calcium and magnesium ions cause hard water. Hard water is not dangerous to health but will cause a build-up of minerals in pipes, anywhere water is heated, such as boilers, kettles and washing machines, and anywhere water has evaporated. This build-up is commonly referred to as limescale.

Also, hard water requires more soap or detergent to create a lather. EDTA sequesters the calcium and magnesium ions so that they do not form limescale precipitates in boilers and washing machines and do not reduce the effectiveness of soaps and detergents.

Cosmetics and Shampoos

EDTA commonly appears on the list of ingredients of shampoos and cosmetics as disodium EDTA. It works as a stabiliser and can improve the cleaning abilities of such products by binding heavy metal ions contained in tap water (see above). It also prevents the metals from being deposited onto the skin and hair.

Additionally, by deactivating the metal ions, cosmetic products will not deteriorate, thereby prolonging their life.

Food Preservation

Calcium disodium EDTA has the E number E385. It is commonly used in mayonnaise, salad dressings, margarines and many carbonated soft drinks. It inhibits the decomposition of oils and fats and prevents them turning rancid. EDTA sequesters trace elements, such as copper, which catalyse the oxidation reactions that cause this decomposition.

Veterinary Medicine

Corneal ulcers are one of the most common eye diseases in dogs. The outer layer of the cornea is lost and results in eye pain causing the dog to squint and paw at the eye. EDTA works by preventing collagenase enzymes breaking down the peptide bonds in collagen, a key component of the cornea.

Health Effects of EDTA

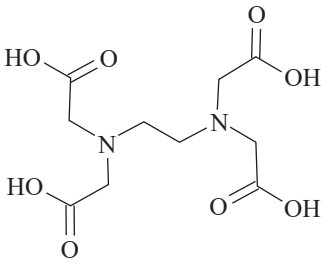
Tests show that standard concentrations of EDTA used in food preservation and cosmetic preparations do not irritate the skin. It is non-carcinogenic and non-toxic. Very large doses are potentially associated with some side effects due to the sequestering by EDTA of metal ions that are needed for normal development.

Question

6 Summarise the uses of EDTA.

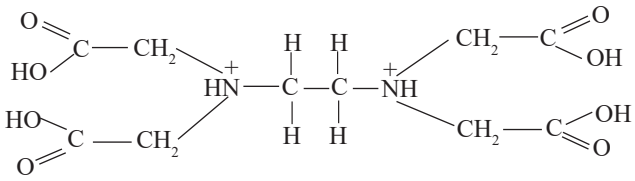
Answers

1.



2. $EDTA + 4NaOH \rightarrow (Na^+)_4EDTA^{4-} + 4H_2O$
   $C_{10}H_{16}N_2O_8 + 4NaOH \rightarrow (Na^+)_4(C_{10}H_{12}N_2O_8)^{4-} + 4H_2O$

3. 2 protons from the acid molecules will form dative covalent bonds to the nitrogen atoms of EDTA to form H_2EDTA^{2+}



4. Aqueous Cu^{2+} ions will be in a complex with six water ligands - $[Cu(H_2O)_6]^{2+}$
   The six neutral water ligands will be substituted by one $EDTA^{4-}$ ligand making the final complex 2- charged.

   $[Cu(H_2O)_6]^{2+} + EDTA^{4-} \rightarrow [CuEDTA]^{2-} + 6H_2O$

5. The $[CuEDTA]^{2-}$ complex is more stable due to the positive entropy change of the substitution reaction. Two reactants form seven reactants. This gives a greater opportunity for disorder; the products will have a higher total entropy than the reactants so the reaction will have a positive entropy change – or answer in terms of ΔG being negative!

6.

Treating lead poisoning	EDTA sequesters Pb^{2+} ions and removes them from the body.
Blood analysis	EDTA stops coagulation of the blood by sequestering Ca^{2+} ions needed for blood clotting.
Treating water hardness	EDTA sequesters Ca^{2+} and Mg^{2+} ions, preventing limescale.
Personal Care Products	EDTA sequesters Ca^{2+} ions and other heavy metals and prevents them being deposited on the skin and hair.
Food preservation	EDTA sequesters Cu^{2+} ions, preventing the catalysis of oxidation of oils and fats.
Animal Care	EDTA sequesters metal ions that would otherwise activate collagenase enzymes and cause breakdown of collagen in the cornea.

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