Technical Information

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Trilon® B types

Trilon® BS
Trilon® B Liquid
Trilon® B Powder
Trilon® BD
Trilon® BX Liquid
Trilon® BX Powder

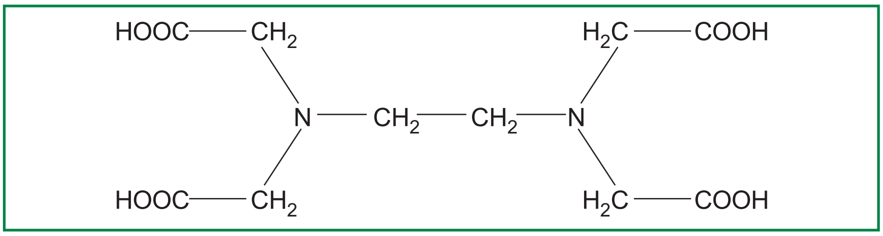
Organic chelating agents used to control the concentration of metal ions in aqueous systems

BASF
The Chemical Company

Chemical nature

The active ingredient contained in the Trilon® B types isethylenediaminetetraacetic acid (EDTA or EDTA-H_4) or its salts.

Ethylenediaminetetraacetic acid, $C_{10}H_{16}N_2O_8$, is an aminocarboxylic acid with six functional groups.



Trilon® BS

Ethylenediaminetetraacetic acid (EDTA-H_4) in solid form
CAS-No. 60-00-4

Trilon® B Liquid

Aqueous solution of the tetrasodium salt of ethylenediaminetetraacetic acid (EDTA-Na_4)
CAS-No. 64-02-8

Trilon® B Powder

Tetrasodium salt of ethylenediaminetetraacetic acid (EDTA-Na_4) in solid form
CAS-No. 64-02-8

Trilon® BD

Disodium salt of ethylenediaminetetraacetic acid (EDTA-H_2Na_2) in solid form
CAS-No. 139-33-3 (Trilon® BD is a dihydrate and has therefore also been assigned CAS-No. 6381-92-6)

Trilon® BX Liquid

Aqueous solution of the tetrasodium salt of ethylenediaminetetraacetic acid (EDTA-Na_4), high purity grade
CAS-No. 64-02-8

Trilon® BX Powder

Tetrasodium salt of ethylenediaminetetraacetic acid (EDTA-Na_4) in solid form, high purity grade
CAS-No. 64-02-8

PRD-Nos.*

30043449	Trilon® BS
30043499	Trilon® B Liquid
30043442	Trilon® B Powder
30043452	Trilon® BD
30043447	Trilon® BX Liquid
30043448	Trilon® BX Powder

* BASF’s commercial product numbers.

Properties

Trilon®	Unit	BS	B Liquid	B Powder
Physical form (visual)		White powder	Clear, yellowish liquid	Slightly yellowish powder
Molar mass	g/mol	292	380	380
Concentration (BASF method)*				
expressed as tetrasodium salt (EDTA-Na_4)	%	–	approx. 40	approx. 87
expressed as free acid (EDTA-H_4)	%	approx. 100	approx. 31	approx. 67
Density (DIN 51757, 20 °C, U-tube densitometer)	g/cm^3	–	approx. 1.31	–
Bulk density (DIN ISO 697, 40 mm diam.)	g/l	approx. 820	–	approx. 690
pH value (DIN 19268, 23 °C, 1% in distilled water)		approx. 2.8 (slurry)	approx. 11.5	approx. 11.5
Hazen color (DIN EN 1557)		–	max. 150	max. 150 (40% in water)
Volatile NH_3 (BASF method)	ppm	–	max. 80	–
Calcium binding capacity (BASF method, pH 11)	mg $CaCO_3$/g t.q.	approx. 350	approx. 110	approx. 235
Water content (DIN EN 13267)	%	approx. 0.1	approx. 57	approx. 7
Viscosity (DIN EN 12092, 23 °C)	mPa·s	–	approx. 25	–
Freezing point (DIN 3013)	°C	–	<-30	–
Melting point (DIN 51004)	°C	approx. 245	–	>300 (decomposes)
Solubility in water (BASF method, 25 °C)	g in 1 liter	<1	Miscible in all proportions	approx. 950

The above information is correct at the time of going to press. It does not necessarily form part of the product specification.

* *Determined by potentiometric titration against iron(III)chloride.*

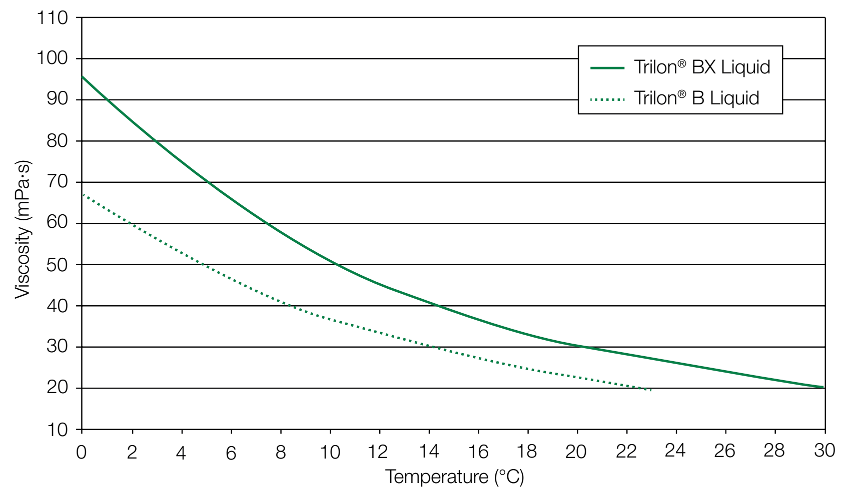
Trilon®	**Unit**	**BD**	**BX Liquid**	**BX Powder**
Physical form (visual)		White powder	Clear yellowish liquid	White, crystalline powder
Molar mass	g/mol	336	380	380
Concentration (BASF method)*				
expressed as tetrasodium salt ($EDTA\text{-}Na_4$)	%	approx. 90	approx. 40	approx. 84
expressed as free acid ($EDTA\text{-}H_4$)	%	approx. 78	approx. 31	approx. 65
Density (DIN 51757, 20 °C, U-tube densitometer)	g/cm^3	–	approx. 1.28	–
Bulk density (DIN ISO 697, 40 mm diam.)		approx. 950	–	approx. 845
pH value (DIN 19268, 23 °C, 1% in distilled water)	g/l	approx. 4.5	approx. 11.5	approx. 11.2
Hazen color (DIN EN 1557)		–	max. 150	max. 50 (40% in water)
Volatile NH_3 (BASF method)	ppm	–	max. 80	–
Calcium binding capacity (BASF method, pH 11)	mg $CaCO_3$/g t.q.	approx. 275	approx. 110	approx. 230
Water content (DIN EN 13267)	%	approx. 10	approx. 60	approx. 16
Viscosity (DIN EN 12092, 23 °C)	mPa·s	–	approx. 20	–
Freezing point (DIN 3013)	°C	–	<-20	–
Melting point (DIN 51004)	°C	approx. 245	–	>300 (decomposes)
Solubility in water (BASF method, 25 °C)	g in 1 liter	approx. 100	Miscible in all proportions	approx. 950

A detailed product specification is available from your local BASF representative.

* *Determined by potentiometric titration against iron(III)chloride.*

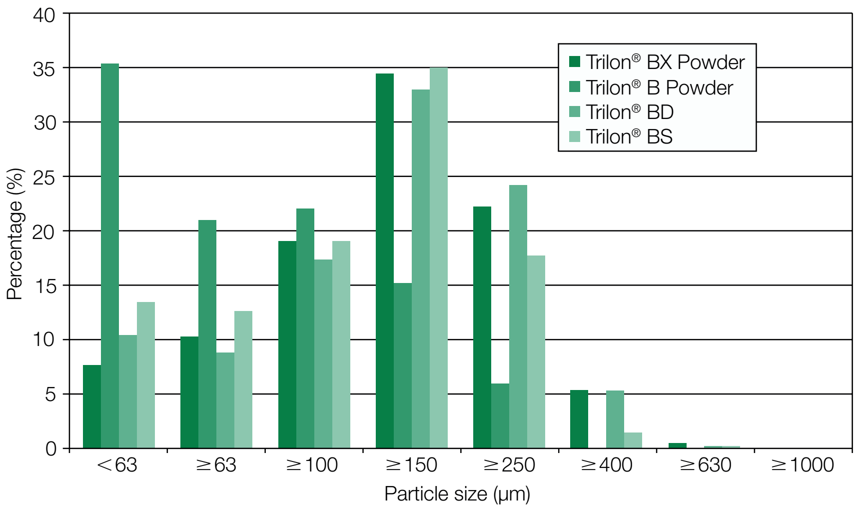
Viscosity

The relationship between viscosity and temperature is always an important point to consider when Trilon® B liquid types are to be delivered or put into storage. The following curve shows the viscosity as a function of temperature. (all values are approximate; mPa·s, Brookfield LVT):



Distribution of particles

The following curve shows the distribution of particles of Trilon® B solid types (all values are approximate):



Complex formation

The most important property of the Trilon® B types is their ability to form water-soluble complexes with polyvalent ions (e.g. calcium, magnesium, lead, copper, zinc, cadmium, mercury, manganese, iron, aluminium) over a wide pH range from 2 to 13.5. EDTA usually forms 1 : 1 complexes, i.e. 1 mol of EDTA chelates binds to 1 mol of metal ions. The metal ion is completely enclosed by the ligand. These complexes remain stable, especially in alkali media and even at temperatures of up to 100 °C.

EDTA has six donor groups and it can form octahedral complexes.

From the law of mass action, the equation for the stability constant K can be written as follows:

$$K = \frac{[MeZ^{(m-n)-}]}{[Me^{n+}]\,[Z^{m-}]}$$

where

$[MeZ^{(m-n)-}]$ is the concentration of the chelate that is formed

$[Me^{n+}]$ is the concentration of free, positively charged metal ions

$[Z^{m-}]$ is the concentration of the ligand anion, in this case EDTA

K is the stability constant for the chelate.

Logarithmic stability constants (log K) for complexes of EDTA and selected metal ions

Metal ion	log K
Co^{3+}	41.0
Fe^{3+}	25.1
Hg^{2+}	21.8
Cu^{2+}	18.8
Ni^{2+}	18.6
Pb^{2+}	18.0
Cd^{2+}	16.5
Zn^{2+}	16.5
Co^{2+}	16.3
Al^{3+}	16.1
Fe^{2+}	14.3
Mn^{2+}	13.8
Ca^{2+}	10.6
Mg^{2+}	8.7
Ba^{2+}	7.9
Ag^{+}	7.3

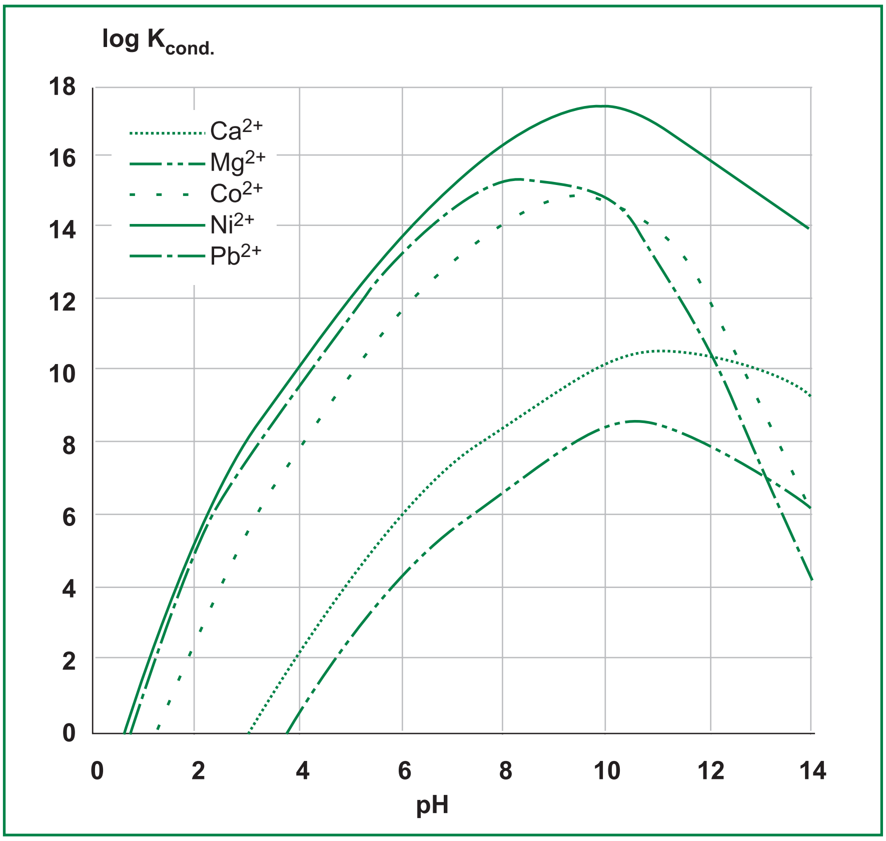
$EDTA\text{-}H_4$ is a tetrabasic acid that dissociates in four steps. The acid dissociation constants pKa are as follows.

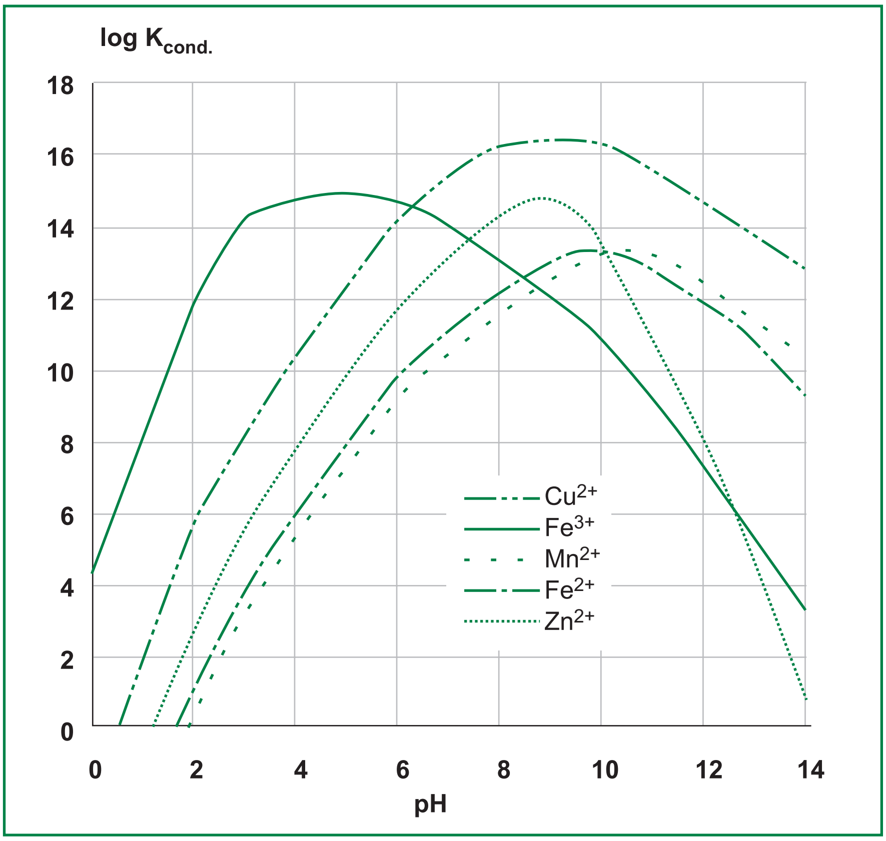
$EDTA\text{-}H_4$	pK_a1	2.0
$EDTA\text{-}H_3^-$	pK_a2	2.6
$EDTA\text{-}H_2^{2-}$	pK_a3	6.2
$EDTA\text{-}H_3^-$	pK_a4	10.3

In aqueous solutions, EDTA competes for metal ions with other anions such as hydroxide, sulphate, sulphide, carbonate and oxalate that form sparingly soluble metal salts. The formation of chelates reduces the concentration of free metal ions $[Me^{n+}]$ to such an extent that the solubility products of many sparingly soluble metal salts are no longer exceeded. The result is that the salts no longer precipitate or may even redissolve.

The high stability of these complexes prevents metal ions from participating in typical chemical reactions. For instance, manganese, iron and copper are no longer able to catalyse the decomposition of peroxide bleach.

Conditional stability constants [log K_{cond}] take into account the stability constant K as well as the acid base dissociation equilibria.





Conditional stability constants for selected EDTA chelates.

The following table shows the amounts in grams of various different bases required to neutralize 100 g of Trilon® BS.

Base	Degree of neutralization			
	1	2	3	4
Sodium hydroxide	13.7	27.4	41.1	54.8
Sodium hydroxide	18.5	37.0	55.5	74.0
Potassium hydroxide	19.2	38.4	57.6	76.8
Ammonia	11.6	23.2	34.8	–
Monoethanolamine (Molar mass 61)	20.8	41.6	62.4	–
Diethanolamine (Molar mass 105)	36.0	72.0	108.0	–
Triethanolamine (Molar mass 149)	51.2	102.4	–	–
N-Diethylethanolamine (Molar mass 117)	40.2	80.4	120.6	–
Oleylamine (Molar mass 267.5)	91.4	182.8	–	–

The table below shows the pH ranges in which EDTA forms complexes.

1 g of $EDTA\text{-}Na_4$ or 0.77 g of $EDTA\text{-}H_4$ are able to sequester the following amounts of metal ions, independently of temperature.

mg	Metal ion	Oxidationnumber	pH range	Color of complex
64	Magnesium	2	8.0 – 12.5	Colorless
105	Calcium	2	6.0 – 13.5	Colorless
230	Strontium	2	8.0 – 13.5	Colorless
361	Barium	2	10.0 – 13.0	Colorless
144	Manganese	2	5.0 – 11.0	Colorless
			5.0 – 13.0*	
147	Iron	2	1.0 – 12.5*	Colorless
154	Nickel	2	1.5 – 13.0	Blue
155	Cobalt	2	4.0 – 12.0	Red**
			4.0 – 13.5	Violet***
167	Copper	2	1.5 – 11.5	Blue
			5.0 – 13.0*	
172	Zinc	2	4.0 – 13.0	Colorless
296	Cadmium	2	3.5 – 13.0	Colorless
545	Lead	2	2.0 – 13.5	Colorless
71	Aluminium	3	2.5 – 13.5	Colorless
138	Chromium	3	1.5 – 5.0	Violet
147	Iron	3	1.0 – 5.5	Yellow
550	Bismuth	3	1.0 – 9.0	Colorless

* *In the presence of a reducing agent*
** *At room temperature*
*** *Appears when heated, persists on cooling*

Chemical stability

The Trilon® B types are chemically very stable.

The Trilon® B types have been shown to be very stable compared to other organic complexing agents such as citric acid, tartaric acid and gluconates, especially at high temperatures.

Whereas inorganic sequestring agents (eg. phosphates) may hydrolyse at high temperatures, Trilon® B types are stable – even when heated to 200 °C under pressure.

Trilon® BS and Trilon® BD melt at approx. 245 °C.

Trilon® B Powder and Trilon® BX gradually lose their water of crystallization at high temperatures and they begin to decompose at approx. 300 °C.

The Trilon® B types are resistant to strong acids and bases. They are gradually broken down by chromic acid, potassium permanganate and other strong oxidizing agents. Stability in the presence of hydrogen peroxide, percarbonate and perborate is sufficient for joint application. Nevertheless, we do not recommend combining Trilon® B types and peroxides in liquid formulations.

Substances that release chlorine, such as sodium hypochlorite, have a highly detrimental effect on the performance of all of the Trilon® B types, and some alkaline earth and heavy metal complexes are broken down.

Corrosion

The Trilon® B types stabilize polyvalent metal ions, which means that they can increase the rate at which metals dissolve. Nevertheless, with the exception of aluminium, an oxidizing agent such as air always has to be present for corrosion to take place. Unalloyed steel is prone to corrosion in media that contain air, but corrosion can be reduced substantially if the pH is in the alkaline range and can be eliminated almost completely if oxygen and other oxidizing agents are excluded. With the exception of aluminium, metals that are cleaned with the Trilon® B types in the slightly alkaline range, which is the optimum pH range for the Trilon® B types, are much less prone to corrosion than if they are cleaned with acids.

The Trilon® B types are capable of dissolving metal oxides such as magnetite, and great caution should be taken in cases in which resistance to corrosion depends the formation of a passive magnetite layer.

The only type of corrosion that has been observed with the Trilon® B types is uniform corrosion: pitting or stress cracking have not been observed in media with a low chloride content. One of the advantages of the Trilon® B types is that they can be supplied with a very low chloride content (<20 mg/kg).

The following information on materials is of a very general nature, because corrosion depends on many different factors such as exposure to air, galvanic corrosion caused by the presence of different materials and by the flow patterns of liquids. The compatibility of Trilon® B types with different materials needs to be tested in each individual case.

Austenitic stainless steels such as AISI/SAE 321 are very effective for vessels used to store and transport the Trilon® B types even at temperatures of 60 – 100 °C.

Ferritic carbon steels such as ASTM A201 Grade B (European Material No. P265GH) are resistant to Trilon® BX Liquid at temperatures up to 60 °C if the liquid is blanketed with nitrogen.

The use of Trilon® BD for cleaning copper components in power stations has been documented in the literature and very little corrosion has been detected even at high temperatures [15].

Aluminium and aluminium alloys such as AL 7075 T6 (European Material No. 3.4365) are not resistant to the Trilon® B types, because Trilon® B Liquid is alkaline and aluminium is quickly corroded by strong bases. The rate of corrosion depends to a large extent on the pH. The neutral and slightly acidic product Trilon® BD is much less corrosive to aluminium than the alkaline Trilon® B types.
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Storage

a) Trilon® B Liquid and Trilon® BX Liquid should not be stored at temperatures below 0 °C, because this can cause them to precipitate. It can be reconstituted by heating it briefly to 40 – 50 °C and stirring.
b) Trilon® B Liquid and Trilon® BX Liquid are easily capable of being pumped at temperatures down to 0 °C.
c) Trilon® B Powder is hygroscopic and soluble in water, with the result that it absorbs moisture very quickly. Drums should be tightly resealed each time material is taken from them.

Materials

The following materials can be used for tanks and drums:

a) AISI 321 stainless steel (X6 CrNiTi 1810)
b) AISI 316 Ti stainless steel (X6 CrNiMoTi 17122)

Shelf life

Trilon® BS and Trilon® BD have a shelf life of three years, provided they are stored in their original packaging and kept tightly sealed.

Trilon® B Liquid, Trilon® BX Liquid and Trilon® BX Powder have a shelf life of two years, provided they are stored in their original packaging and kept tightly sealed.

Trilon® B Powder has a shelf life of 18 months, provided it is stored in its original packaging and kept tightly sealed.

Ecological and Toxicological Data

The toxicological and ecological properties of EDTA have been evaluated in detail by the authorities of the European Community [1]. In addition, publicly accessible documents include the report by the Dutch Institute for Health and Environment [2] and the WHO Guidelines for drinking-water quality [3].

EDTA does not fulfill the criteria of easy biological degradability according to standard OECD tests, yet biological decomposition has been proven under suitable conditions – higher retention times, low alkaline pH, or adapted bacterial flora [1, 4a, 4b], i.e., conditions that are found in nature. Biological decomposition was also proven directly for EDTA complexes – calcium, manganese, and zinc [5, 6].

Photochemical decomposition of the EDTA complexes of iron, cobalt, and manganese is also known [1], and FeEDTA in particular is significantly present in the environment under slightly acidic conditions [7]. Photooxidation of EDTA under real conditions – natural river water with no deliberate addition of iron, natural sunlight – has also been confirmed on numerous occasions [7, 8, 9].

EDTA has been reported within the ppb range in many waters in Europe. However, the amounts found in the environment are clearly lower than the amount used [1]. This can be explained by the proven photochemical and biological decomposition. As described under REACH, EDTA can be evaluated as "widely biologically degradable" [10].

EDTA is not to be classified as "persistent," according to REACH.

Furthermore, EDTA can be destroyed directly in wastewater treatment by UV oxidation [11].

EDTA only has low aquatic toxicity; within the EU risk assessment, a PNEC of 2,200 µg/L was established. This value is approx. 100–1,000-fold above presently typical values for EU waters [1].
The remobilization of heavy metals by EDTA has been intensively discussed and evaluated. It is only conceivable under extreme conditions, given that the exchange of metals proceeds relatively slowly. EDTA is preferentially found in the water phase low in heavy metals, and hardly at all in the sediment phase rich in heavy metals; heavy metals frequently occur tightly bound in the environment. Typically, the respective metal complex already forms when EDTA is used, at the latest in the wastewater system, where ZnEDTA frequently predominates. No correlation between EDTA and heavy-metal content of waters in the environment could be proven [1, 7, 12].

The absorption of EDTA across the food chain should also be evaluated as uncritical. EDTA is a toxicologically well evaluated substance [1] and has been used medically in chelation therapy for many decades. It is not easily absorbed by the digestive tract and quickly excreted through the urine [13, 14]. In many countries, EDTA is permitted as a food additive.

Due to its high polarity and good water solubility, it does not accumulate in the food chain, and the amounts absorbed through food and drinking water are typically 1.000-fold under digestible amounts.

Safety

We know of no ill effects that could have resulted from using the Trilon® B types for the purpose for which they are intended and from processing them in accordance with current practice.

According to the experience we have gained over many years and other information at our disposal, the Trilon® B types do not exert any harmful effects on health, provided that they are used properly, due attention is given to the precautions necessary for handling chemicals, and the information and advice given in our safety data sheets are observed.

Please refer to the latest Safety Data Sheets for detailed, up-to-date information on classification, labelling and product safety.

Literature

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Note

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