

## Technical Information

**Neutrol® MGDA**

PRD 30757117

Valid since 23.06.2020  
Revision 1.0

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**Care Chemicals****Complexing Agent****INCI name(s)**

Trisodium Dicarboxymethyl Alaninate

**Chemical description**

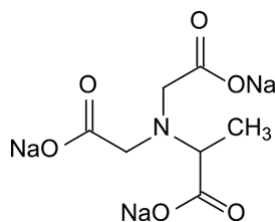
Trisodium salt of methylglycinediacetic acid

**Physical form:**

Fine yellow powder at room temperature

**Molecular weight**

271 g/mol

**Molecular Formula**C<sub>7</sub>H<sub>8</sub>NNa<sub>3</sub>O<sub>6</sub>**Structural Formula****CASR-No.**

164462-16-2

**Ingredient**

Alanine, N,N-bis(carboxymethyl)-, trisodium salt

**Characteristic values**

The specifications stated in the paragraphs 'Quality control data' and 'Additional product descriptive data' finally and conclusively describe the properties of the product.

**Quality control data**

(Data which is used for quality release and is certified for each batch.)

**Test property**Concentration calculate as MGDA-  
Na<sub>3</sub> (molecular weight MW 271 g/  
mol)

pH value (25 °C; 1 % in water)

Bulk density

**Specification**

85 - 88 %

10.5 - 12.5

670 - 820 g/l

**Test method**Internal method (pot. titration with  
FeCL<sub>3</sub>-solution)

DIN 19268

DIN ISO 697

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### Additional product descriptive data

(Data which is proven statistically but not determined regularly.)

Test property	Specification	Test method
NTA content	max. 0.1 %	Internal method

## Storage information

### Shelf life

12 months

### Storage temperature

Store in a dry place below approx. + 50 °C. The product must be stored moisture-free since it is very hygroscopic. Opened containers should be resealed tightly after each removal of product to prevent absorption of moisture.

### Storage conditions

In original sealed containers and protected from moisture

## Stabilising additives / Auxiliaries

### Preservatives

not present

### Antioxidants

not present

### Solvents

not present

### Others

not present

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## Composition hints for finished product label

### INCI Components

**INCI Name (US/EU/CN)**

Trisodium Dicarboxymethyl Alaninate

**Content**

85 - 88 %

### Water Content

**Content**

12 - 15 %

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### Specific technical data

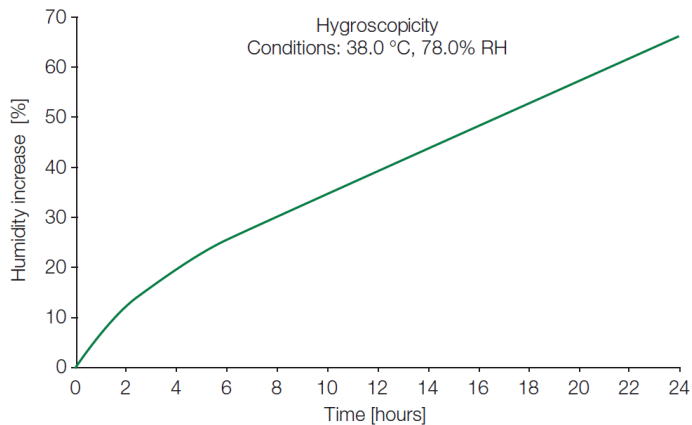
#### Appearance

Fine yellow powder at room temperature:



#### Hygroscopicity

For storage and processing of Neutrol® MGDA it is important to know how the product behaves at elevated temperatures and humidity. The following graph shows this dependency (the represent approximate values):



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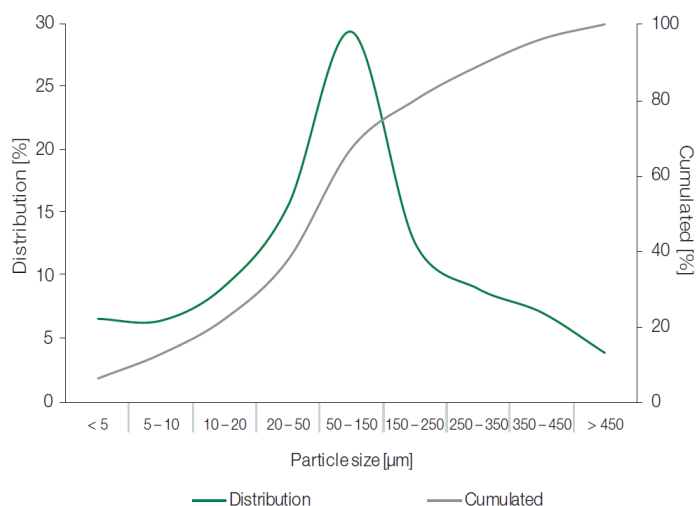
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**Particle size distribution**



**Complex formation**

The most important property of Neutrol® MGDA is the ability to form watersoluble complexes with polyvalent ions (e.g., calcium, magnesium, lead, copper, zinc, cadmium, mercury, manganese, iron) over a wide pH range (from 2 to 13.5).

MGDA usually forms 1 : 1 complexes, i. e. 1 mol of MGDA chelates binds 1 mol of metal ions. The complexes remain stable, especially in alkaline media and, even at temperatures of up to 100 °C.

From the law of mass action, the equation for the stability constant K for 1 : 1 complexes can be written as follows:

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

where

$[MeZ^{(m-n)}]$  is the concentration of the formed metal complex,

$[Me^{n+}]$  is the concentration of the free metal ion, with  $Me^{n+}$  being a positively charged metal ion,

$[Z^{m-}]$  is the concentration of the chelating agent anion (MGDA), and

K is the chelate formation constant of the metal complex.

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Logarithms of the chelate formation constant (log K) of a number of MGDA/metal ion complexes:

Metal ion	log K
Fe <sup>3+</sup>	16.5
Cu <sup>2+</sup>	13.9
Pb <sup>2+</sup>	12.1
Ni <sup>2+</sup>	12.0
Co <sup>2+</sup>	11.1
Zn <sup>2+</sup>	10.9
Cd <sup>2+</sup>	10.6
Mn <sup>2+</sup>	8.1
Fe <sup>2+</sup>	8.4
Ca <sup>2+</sup>	7.0
Mg <sup>2+</sup>	5.8
Sr <sup>2+</sup>	5.2
Ba <sup>2+</sup>	4.9

A high value for log K indicates that the chelating agent has a high affinity for that particular metal ion, and it provides a preliminary indication of whether the chelating agent is suitable for the specific application. MGDA-H3 is a tribasic acid that dissociates in three steps.

The pKa values are as follows:

MGDA-H <sub>3</sub>	pK <sub>a1</sub>	1.6
MGDA-H <sub>2</sub> <sup>-</sup>	pK <sub>a2</sub>	2.5
MGDA-H <sup>2-</sup>	pK <sub>a3</sub>	10.0

In aqueous solutions, MGDA 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<sup>n+</sup>] 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 the complexes prevents the typical reactions of the metal ion. This leads to the suppression of the manganese-, iron- or copper-catalyzed decomposition of peroxidic bleaches, for instance.

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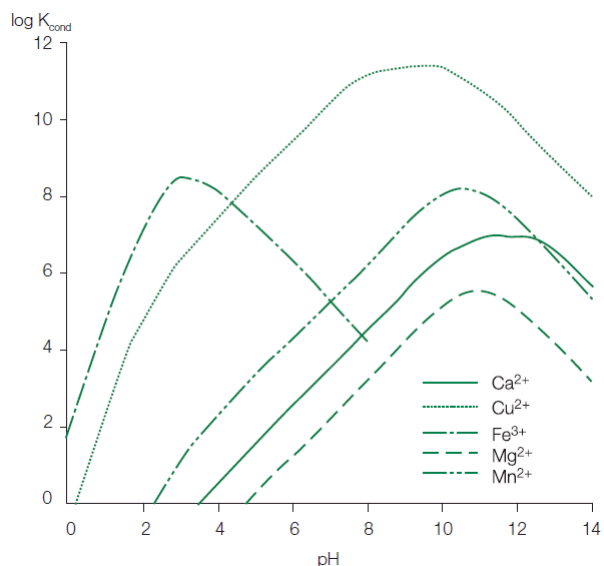
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Besides the log K value, the conditional stability constants [ $\log K_{\text{cond}}$ ] might also help in choosing the proper chelating agent for an application. In addition, these take into consideration the acid-base dissociation equilibria of chelating agent and complex in water and therefore the effect of the pH value on the complex.



Conditional stability constants for the most important MGDA metal complexes.

**Chemical stability**

- Neutrol® MGDA is highly stable compared with other organic chelating agents (e.g. citric acid, tartaric acid, gluconate), especially at high temperatures
- Neutrol® MGDA is neither decomposed by strong acids nor by strong bases
- Neutrol® MGDA is sufficiently stable to hydrogen peroxide
- Neutrol® MGDA generally stabilizes multivalent metal ions and might accelerate the dissolving behavior of metals through chelate formation

**Ecology and toxicology**

- Neutrol® MGDA has outstanding ecological (ecotoxicological) and toxicological properties.
- The active ingredient in Neutrol® MGDA, is classified as readily biodegradable based on OECD standards. This means that Neutrol® MGDA, in such a test, for example, is degraded into water and its mineral components by the microorganisms present in wastewater treatment plants.

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The products supplied by BASF conform to stringent standards with respect to their toxicological and ecotoxicological properties in order to provide protection of human and the environment

**Miscellaneous information****Chemical Nature**

Neutrol® MGDA is the trisodium salt of methylglycinediacetic acid (MGDA-Na<sub>3</sub>)

Methylglycinediacetic acid is also referred to as alpha-alaninediacetic acid.

Methylglycinediacetic acid, is an aminocarboxylic acid containing four functional groups, that can chelate metal ions.

**Performance**

Readily biodegradable Neutrol® MGDA is a new offering of BASF in addition to the strong chelating agents of the Edeta® product line.

**Intended for use as cosmetic ingredient****Disclaimer**

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