

TRISODIUM NITRILOTRIACETATE

Part I - Environment

CAS No: 5064-31-3

EINECS No: 225-768-6

Summary Risk Assessment Report

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SUMMARY RISK ASSESSMENT REPORT

Final report, 2005

Germany

The risk assessment of trisodium nitrilotriacetate has been prepared by Germany on behalf of the European Union.

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PREFACE

This report provides a summary, with conclusions, of the risk assessment report of the substance trisodium nitrilotriacetate (Part I-Environment) that has been prepared by Germany in the context of Council Regulation (EEC) No. 793/93 on the evaluation and control of existing substances.

For detailed information on the risk assessment principles and procedures followed, the underlying data and the literature references the reader is referred to the comprehensive Final Risk Assessment Report (Final RAR, Part I-Environment) that can be obtained from the European Chemicals Bureau¹. The Final RAR should be used for citation purposes rather than this present Summary Report.

¹ European Chemicals Bureau – Existing Chemicals – <http://ecb.jrc.it>

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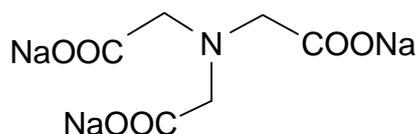
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1 GENERAL SUBSTANCE INFORMATION

1.1 IDENTIFICATION OF THE SUBSTANCE

CAS No: 5064-31-3
EINECS No: 225-768-6
IUPAC Name: Trisodium nitrilotriacetate
Synonyms: Nitrilotriacetic acid trisodium salt, NTA trisodium salt
CA Index name: Glycine, N,N-bis(carboxymethyl)-, trisodium salt
Empirical formula: $C_6H_6NNa_3O_6$
Molecular weight: 257.1 g/mol
Structural formula:



1.2 PURITY/IMPURITIES, ADDITIVES

Purity: $\geq 92\%$ w/w
Impurity: < 7% water
< 3 sodium glycolate
< 2% disodium iminodi(acetate)
< 2 sodium hydroxide
< 1,5% methanamine
< 1 sodium formate
Additives: none

1.3 PHYSICO-CHEMICAL PROPERTIES

Trisodium nitrilotriacetate (Na_3NTA) is a colourless crystalline powder at room temperature and normal pressure. Data on the physical and chemical properties are given in **Table 1.1**.

Table 1.1 Physico-chemical properties

Parameter	Value
Melting point	410°C with decomposition above 200°C
Boiling point	not applicable
Relative density	1.77 at 20°C
Vapour pressure	not determined
Surface tension	not determined
Water solubility	about 640 g/l at 20°C
Partition coefficient	-2.62 (calculated)
Flash point	not determined
Flammability	not highly flammable
Ignition temperature	no self ignition up to decomposition (200°C)
Explosive properties	not explosive
Oxidising properties	no oxidising properties

1.4 CLASSIFICATION

Classification according to Annex I

Class of danger: none

R-Phrase: none

The classification of NTA is not included in Annex I to Directive 67/548/EEC.

Proposed classification (only environmental part)

For the classification of biodegradation, the available laboratory tests with uncomplexed NTA should not be used, because biodegradation of this chelator is strongly dependent on the metal speciation. Studies on the degradation in biological treatment plants as well as degradation tests conducted in river water reveal that the degradation properties of NTA (its metal complexes respectively) are comparable with a readily degradable substance. In addition the substance has no bioaccumulation potential.

In tests on the acute toxicity on fish and daphnia effects were only observed when NTA was present in over-stoichiometric concentrations compared to the content of metal ions. The lowest LC₅₀ values were 98 mg/l for both trophic levels.

Results of algae growth inhibition tests have to be interpreted carefully, because the observed effects are mainly caused by nutrient deficiency, which is an artefact and not relevant for the environment. Tests with increased concentrations of nutrient metals (where nutrient deficiency is suppressed) reveal that intrinsic toxicity of NTA is expected only at concentrations far above 10 mg/l.

Considering all results, a classification of Na₃NTA for the environment is not recommended.

2 GENERAL INFORMATION ON EXPOSURE

2.1 PREMARK

Nitrilotriacetate is produced and used as sodium salt (Na_3NTA) or as acid (H_3NTA). During the use and, after release into the environment, complexes with metal ions are formed. The environmental exposure of all NTA complex species is overlapping. In the scientific literature dealing with the environmental fate and toxic effects on organisms, amounts and concentrations are mostly referred to Na_3NTA . Thus, for the environmental risk assessment all production and use volumes are given as Na_3NTA equivalents, abbreviated NTA throughout the document.

2.2 PRODUCTION

Four companies are reported as producing NTA. A total quantity of 26,642 tonnes/annum was marketed in 2000 within the EU.

NTA can be produced by a one-stage alkaline process which is based on the cyanomethylation of ammonia (or ammonium sulfate) with formaldehyde and sodium cyanide (or hydrogen cyanide).

Another possibility to produce NTA is a two-stage acidic process which features much lower by-product levels. In the first stage, ammonia is reacted with formaldehyde to give hexamethylenetetramine, which is then reacted with hydrogen cyanide in sulfuric acid solution to yield triscyanomethylamine. The solid triscyanomethylamine is sparingly soluble in the acidic solution and is filtered off, washed, and saponified with NaOH to give Na_3NTA .

2.3 USE PATTERN

NTA is an aminocarboxylic acid with three functional groups which donate electrons. These enable it to participate in complexation reactions. The most important property of NTA is to form water-soluble complexes with multivalent metal ions over a wide pH range.

NTA and its sodium salt are used to soften water and to remove traces of alkaline earth and heavy metals. They are often included in detergent and cleaner formulations for household or industrial use (67%). About 4% is used in textile cleaning. The use of almost a third of the total market volume could not further be specified.

3 ENVIRONMENT

3.1 ENVIRONMENTAL EXPOSURE

3.1.1 General discussion

Releases of NTA occur during production and use via waste water into the hydrosphere.

Degradation

In a series of laboratory degradation tests NTA was readily degraded (complete mineralisation). Accumulation of a stable metabolite is not expected. In most cases the acid or the Na-salt was added and not the complexed NTA. However, the test media generally contain, beside trace metals, calcium and/or magnesium ions in over-stoichiometric amounts. The respective complexes are formed being the active test substances. For the environmental exposure assessment, the degradation properties of the metal complexes instead of the uncomplexed agent have to be taken into account.

There are contradicting results about the degradable metal species. These may be caused by specific degradation mechanisms in individual inoculi. There is an agreement that complexes with several heavy metals inhibit NTA degradation. Heavy metals are widely spread; considerable fractions of NTA may be bound to these metals thus influencing the agent's removal in treatment plants and in environmental compartments.

However, non-degradable complex species can be transformed into degradable compounds by metal exchange reactions. As in sewage and the hydrosphere always a mixture of complexes is present, a prediction of the degradation rates from standard laboratory tests is not possible.

Based on studies on removal of NTA in municipal treatment plants a removal of 95% is used for the assessment.

There are studies available demonstrating that NTA is biodegraded in freshwaters with half-life in the range of several hours to some days, after an acclimation period in the range of days to weeks. Degradation is considerably influenced by temperature. For the exposure calculations, a half-life of 5 days is used.

There are some studies on biodegradation in soil available. A half-life of 9 d is used for soils. The same half-life is applied for the aerobic sediment layer. For anaerobic sediments, a roughly estimated half-life of 20 days is assumed.

The available studies demonstrate that in surface waters photolysis can contribute to NTA degradation. However, there are only small fractions of the photolytically instable complex species at thermodynamical equilibrium state. Biodegradation is the predominant degradation mechanism, therefore photolysis is not considered in the exposure assessment.

Distribution

Because of the salt character of NTA no value for the vapour pressure is available.

Due to the ionic structure under environmental relevant pH conditions, a relevant adsorption onto the organic fraction of soils or sediments is not expected. However, interaction with the mineral phase is possible.

Based on an experimental study, a value of K_p of 1.6 l/kg is used for adsorption onto sediments, suspended particles, and soils.

Bioaccumulation

There are various studies on bioaccumulation demonstrating a low accumulation of NTA. For the assessment, a BCF value of 3 l/kg is chosen.

3.1.2 Aquatic compartment (incl. sediment)

3.1.2.1 Production

Exposure scenarios were calculated based on site-specific data of 4 production sites. The calculated PEC_{local} values are in the range from < 5.1 $\mu\text{g/l}$ to 450 $\mu\text{g/l}$.

3.1.2.2 Use

Based on the TGD principles and applying the 10% rule the following STP-effluent concentrations $C_{local,eff}$ (= PEC_{STP}) and $PEC_{s_{aqua}}$ are derived for the identified life cycle stages (see **Table 3.1**)

Table 3.1 Summary of PECs

	PEC_{STP} [$\mu\text{g/l}$]	$PEC_{s_{aqua}}$ [$\mu\text{g/l}$]
Formulation of cleaning agents	450	49
Use of cleaning agents	450	49
Textile cleaning, Formulation	160	20
Textile cleaning, Use	5,000	500
$PEC_{regional}$		4.2

Because of the low partitioning coefficients, no accumulation in sediments is expected. In addition, neither monitoring data nor any tests for sediments are available. If the equilibrium partitioning method is used, the aquatic $PEC/PNEC$ ratios result. Thus an assessment of sediment is not necessary.

There are a number of measured levels of NTA in surface water and waste water available which are generally of the same order of magnitude as the calculated values.

3.1.2.3 NTA metal complexes in the hydrosphere

In natural waters, both natural and anthropogenic metals are present, which are able to form complexes with NTA.

When metal complexes come into contact with other metals, metal exchange reactions occur. Complexes being wasted from any technical process reach a treatment plant and are mixed with other waste waters, leading to a change in the speciation. The same processes occur when the effluent is released into surface waters with a different metal composition. The mechanism of metal exchange reactions is dissociation of a metal complex with subsequent binding of another metal ion. The rate of the exchange reaction is limited by the rate of the

dissociation of the mother complex. The reaction rates vary in a large range. For NTA, reaction rates in the order of hours for Ni and seconds for Zn are quoted.

Raw sewages always contain a more or less high amount of heavy metals. In general heavy metals are strongly adsorbed onto sewage sludge thus being removed from the water phase. By complexation with agents like NTA the metals are kept in the soluble phase. When the chelator is biologically degraded the metal ions are set free and adsorbed. When the chelator is not completely degraded, increased metal concentrations can occur in the effluent.

Therefore, increased heavy metal releases into the hydrosphere can occur with high NTA loads or when NTA degradation is disturbed. Simultaneously, the deloaded sludge leads to less contamination of agricultural soil if sludge is applied as fertiliser.

3.1.3 Atmosphere

No relevant releases into the atmosphere are expected.

3.1.4 Terrestrial compartment

No relevant releases into soils are expected.

3.1.5 Secondary poisoning

From the ionic structure of sodium NTA it can be concluded that a significant accumulation of these substances in the biota is not to be expected.

3.2 EFFECTS ASSESSMENT

3.2.1 Aquatic compartment (incl. sediment)

NTA is always complexed with metal ions if over-stoichiometric amounts of metal ions are present in the environment. These reactions also take place in toxicity test media, where metal ions are complexed when uncomplexed NTA is added. A generally accepted hypothesis is that the toxicological profile of complexing agents is based on disturbances of metal metabolism. It is expected that effects are caused by the uncomplexed agent. This is supported by the increased effect values in hard water.

Acute toxicity test results are reported for fish, invertebrates and algae. Test results on acute toxicity to fish resulted in 96-hour LC₅₀ values in the range of 98 – 487 mg/l. Short-term results for invertebrates range from 79 to > 1,000 mg/l whereby it is not clear whether the lowest concentration refers to H₃NTA or Na₃NTA. For algae, the 96-hour EC_{b50} is 477 mg/l for hard water and 133 mg/l for soft water.

Long-term studies are also reported for fish, invertebrates and algae. The lowest effect value for fish was derived as 54 mg/l (*Pimephales promelas*) based on a 224-day generation cycle test. The NOEC for invertebrates is 9.3 mg/l (*Gammarus pseudolimnaeus*) based on a generation cycle test over 21 weeks exposure. A 5-day NOEC of 5 mg/l was derived for 3 algal species (*Selenastrum capricornutum*, *Scenedesmus subspicatus* and *Chlorella vulgaris*).

The apparent toxicity of complexing agents to algae in standard tests is related to essential trace metal bioavailability. Trace metal levels tend to be more important in algal growth tests than in other short-term tests (e.g. on fish or daphnia); the main reason is the rapid increase of

biomass during the test. In standard tests using uncomplexed agents, the concentrations of free essential metal ions decrease drastically, leading to nutrient deficiency and relatively low effect concentrations.

The studies cited above reveal that the effects are mainly caused by nutrient deficiency. Therefore, the inhibition of algae growth is an artefact which is caused by the drastic increase of biomass during the test. As in the environment metal ions are generally present in over-stoichiometric amounts, nutrient deficiency is not expected.

There is a study on pond ecosystems available showing neither nutrient deficiency nor eutrophication at concentrations of up to 500 $\mu\text{g/l}$ H_3NTA (= 670 $\mu\text{g/l}$ Na_3NTA).

Based on all available data a $\text{PNEC}_{\text{aqua}}$ of 0.93 mg/l is derived using an assessment factor of 10.

3.2.2 Toxicity to Microorganisms

The lowest valid effect value is a 72-hour EC_5 of > 540 mg/l (as Na_3NTA) for *Chilomonas paramecium*. A $\text{PNEC}_{\text{microorg.}}$ > 540 mg/l is observed using an assessment factor of 1.

3.2.3 Atmosphere

Because there are no fumigation tests available, an effects assessment for this compartment can not be performed.

3.2.4 Terrestrial compartment

There are no tests on terrestrial organisms available, thus an effects assessment for this compartment can not be performed.

3.2.5 Secondary poisoning

As there is no bioaccumulation, a biomagnification via the food chain is not expected.

3.3 RISK CHARACTERISATION

3.3.1 Aquatic compartment

In the following table, the results for all calculated exposure scenarios are listed:

Table 3.2 Risk characterisation for the aquatic compartment

Scenario	PECaqua / PNECaqua	Ceffl. / PNECmicro
Producer A	Only import	
Producer B	< 0.005	No WWTP
Producer C	0.006	< 0.0001
Producer D	< 0.48	No WWTP
Producer E	0.015	< 0.002
Textile Cleaning, Formulation	0.022	< 0.0003
Textile Cleaning, Use	0.54	< 0.009
Cleaning agents, Formulation	0.053	< 0.0008
Cleaning agents, Use	0.053	< 0.0008

Surface water

There is no indication of a risk to the aquatic compartment. **Conclusion (ii).**

Wastewater treatment plants

There is no indication of a risk to microorganisms. **Conclusion (ii).**

Sediments

There are neither monitoring data for sediments nor toxicity tests with benthic organisms available. The Na₃NTA concentration could be modelled using the equilibrium partitioning method. A risk assessment for sediments would lead to identical PEC/PNEC ratios like for the aquatic compartment.

Because of the low partitioning coefficients, no accumulation in sediments is expected. Thus an assessment of this sub-compartment is not necessary. **Conclusion (ii).**

Influence on the Distribution of Heavy Metals

Significant remobilisation processes of heavy metals from loaded sediments are only expected in extreme cases, i.e. when high NTA amounts are released. This would lead to increased concentrations of those metals with high conditional complex-formation constants. With the concentrations estimated in this risk assessment, those effects are not expected. **Conclusion (ii).**

3.3.2 Atmosphere

No relevant releases into the atmosphere are expected; therefore a risk characterisation for this compartment is not necessary. **Conclusion (ii).**

3.3.3 Terrestrial compartment

No relevant releases into soils are expected; therefore a risk characterisation for the terrestrial compartment is not necessary. **Conclusion (ii).**

3.3.4 Secondary poisoning

As there is no bioaccumulation, a biomagnification via the food chain is not expected.

Conclusion (ii).

4 HUMAN HEALTH

(to be added later)

5 RESULTS

5.1 ENVIRONMENT

Conclusion (ii) There is at present no need for further information and/or testing and no need for risk reduction measures beyond those which are being applied already.

Production and use of Na₃NTA within the EU are examined. The PEC/PNEC ratios are below 1 for all compartments and all life-cycle steps. Therefore, a risk for the environment is not expected.

