

Ecotox Report for Case # P-19-0109

General

Status: 04/24/2020	Report Status: Complete
Date:	CRSS Date: 01/21/2020
SAT Date:	SAT Chair:
Consolidated PMN: N	Consolidated Set:
Ecotox Related Cases:	
Health Related Cases:	
Submitter: Arch Chemicals, Inc.	
CAS Number:	
Chemical Name: Copper, bis[2-(amino-.kappa.N)ethanolato-.kappa.O]-; Copper, [[2,2',2''-(nitrido-.kappa.N)tris[ethanolato-.kappa.O]](2-)]-	
Use: Intended use: Component of a cleaning formulation that is used to improve the wettability of the overall cleaning solution on the substrate.	
	Analogues (same use): None found.
	Patents (same use): None found.
Trade Name: Copper ethanolamine complex, Postur-E (Industrial Product), Cutrine Ultra (FIFRA product)	
PV-max(kg/yr):	Ecotox Corrales, Assessor: Jone

Fate Summary Statement

Fate P-19-0109

Summary FATE:

Statement: Estimations for ethanolamine anion, MW = 61, C₂H₇NO

log Kow = -1.31 (M)

log Koc = 0.07 (E)

log Fish BCF = 0.50 (3) (E)

log Fish BAF = -0.05 (1) (E)

FATE: Estimations for triethanolamine anion, MW = 149, C₆H₁₅NO₃

log Kow = -1.00 (M)

log Koc = 1.00 (E)

log Fish BCF = 0.50 (3) (E)

log Fish BAF = -0.05 (1) (E)

PMN Substance: Solid

S

> 10 g/L at 25 °C (E)

VP < 1.0E-6 torr at 25 °C (E)

BP >

400 °C (E)

H < 1.00E-8 (E)

POTW removal (%) = Anion Ethanolamine

75-90 via biodeg; Anion Triethanolamine 50-90

via biodeg; Cation 75-90

via sorption

Time for complete ultimate aerobic biodeg = Anion

Ethanolamine wk; Anion Triethanolamine

wk; Cation > mo

Sorption

to soils/sediments = Anion Ethanolamine low; Anion Triethanolamine low;

Cation v.strong

PBT Potential: Anion Ethanolamine P1B1; Anion

Triethanolamine P1B1; Cation P3B*(low)

FATE: Migration to ground water

= Anion Ethanolamine moderate; Anion Triethanolamine

moderate; Cation

negl

Bioconcentration factor to be put into E-FAST: Anion Ethanolamine

3.2; Anion

Triethanolamine 0.04; Cation N/A

Analogue data found

(include identifier and database)

Relevant

Structure(s)

Water Anions and Cation

Landfill Anions and

Cation

Air / Incineration Parent

Parent % incineration 0% for the

cation and 99.9% for both anions

Environmental Fate

Determination

PMN #: P-19-0109

Summary: EPA estimated that the

first anion (ethanolamine) could have limited persistence and low

potential for bioaccumulation, such that repeated exposures are not

expected to cause food-chain effects via accumulation in exposed

organisms. EPA estimated that the second anion (triethanolamine) could

have limited persistence and low potential for bioaccumulation, such that

repeated exposures are not expected to cause food-chain effects via

accumulation in exposed organisms. Although EPA estimated that the cation

could be very persistent, the substance does not bioaccumulate by

lipophilic partitioning and there is low concern that it will accumulate

in organisms by other mechanisms; thus, repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

Fate: Environmental fate is the determination of which environmental compartment(s) a chemical moves to, the expected residence time in the environmental compartment(s) and removal and degradation processes. Environmental fate is an important factor in determining exposure and thus in determining whether a chemical may present an unreasonable risk. EPA estimated physical/chemical and fate properties of the first anion (ethanolamine) using data available for the first anion (ethanolamine, CASRN 141-43-5) and EPI (Estimation Program Interface) Suite™

(<http://www.epa.gov/tsca-screening-tools/epi-suite™-estimation-program-interface>), of the second anion (triethanolamine) using data available for the second anion (triethanolamine, CASRN 102-71-6) and EPI (Estimation Program Interface) Suite™

(<http://www.epa.gov/tsca-screening-tools/epi-suite™-estimation-program-interface>), and of the cation using data for analogue(s) (). In wastewater treatment, the first anion (ethanolamine) is expected to be removed with an efficiency of 75% to 90% due to biodegradation, the second anion (triethanolamine) is expected to be removed with an efficiency of 50% to 90% due to biodegradation, and the cation is expected to be removed with an efficiency of 75% to 90% due to sorption. Removal of the first anion (ethanolamine) by biodegradation is high, removal of the second anion (triethanolamine) by biodegradation is moderate to high and removal of the cation by biodegradation is negligible. Sorption of the first anion (ethanolamine) to sludge, soil, and sediment is expected to be low, sorption of the second anion (triethanolamine) to sludge, soil, and sediment is expected to be low, and sorption of the cation to sludge is expected to be strong and to soil and sediment is expected to be very strong. Migration of the first anion (ethanolamine) to groundwater is expected to be moderate due to low sorption to soil and sediment, mitigated by biodegradation, migration of the second anion (triethanolamine) to groundwater is expected to be moderate due to low sorption to soil and sediment, mitigated by biodegradation and migration of the cation to groundwater is expected to be negligible due to very strong sorption to soil and sediment. Due to low estimated vapor pressure and Henry's law constant, the first anion (ethanolamine) and the second anion (triethanolamine) are expected to undergo low volatilization to air and the cation is expected to undergo negligible volatilization to air. Overall, these estimates indicate that the first anion (ethanolamine) and the second anion (triethanolamine) have low potential to volatilize to air and moderate potential to migrate to groundwater and that the cation has low potential to volatilize to air or migrate to groundwater.

Persistence : Persistence is relevant to whether a new chemical substance is likely to present an unreasonable risk because chemicals that are not degraded in the environment at rates that prevent substantial buildup in the environment, and thus increase potential for exposure, may present a risk if the substance presents a hazard to human

health or the environment. EPA estimated degradation half-lives of the first anion (ethanolamine) using data available for the first anion (ethanolamine, CASRN 141-43-5), of the second anion (triethanolamine) using data available for the second anion (triethanolamine, CASRN 102-71-6) and of the cation using data for analogue(s) ([REDACTED]). EPA estimated that the first anion (ethanolamine) and second anion (triethanolamine)'s aerobic and anaerobic biodegradation half-lives are < 2 months; and that the cation's aerobic and anaerobic biodegradation half-lives are > 6 months. These estimates indicate that the first anion (ethanolamine) may have limited persistence in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment). These estimates also indicate that the second anion (triethanolamine) may have limited persistence in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment). Further, these estimates indicate that the cation may be very persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

Bioaccumulation : Bioaccumulation is relevant to whether a new chemical substance is likely to present an unreasonable risk because substances that bioaccumulate in aquatic and/or terrestrial species pose the potential for elevated exposures to humans and other organisms via food chains. EPA estimated the potential for the first anion (ethanolamine) and the second anion (triethanolamine) to bioaccumulate using EPI Suite™; and the potential for the cation to bioaccumulate using data for analogue(s) ([REDACTED]). EPA estimated that the first anion (ethanolamine) has low bioaccumulation potential based on BCFBAF model result < 1000 (first anion (ethanolamine) bioconcentration factor = 3.2 [estimated by linear regression from log Kow] and bioaccumulation factor = 0.9 [estimated by the Arnot-Gobas method (2003)]), while the second anion (triethanolamine) has low bioaccumulation potential based on BCFBAF model result < 1000 (second anion (triethanolamine) bioconcentration factor = 0.4 [measured] and bioaccumulation factor = 0.9 [estimated by the Arnot-Gobas method (2003)]). The cation does not bioaccumulate by lipophilic partitioning and there is low concern that it may accumulate in organisms by other mechanisms. EPA estimated that the first anion (ethanolamine) could have limited persistence and low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. EPA estimated that the second anion (triethanolamine) could have limited persistence and low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. Although EPA estimated that the cation could be very persistent, the substance does not bioaccumulate by lipophilic partitioning and there is low concern that it will accumulate in organisms by other mechanisms; thus, repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

Physical Chemical Information

181.68

Molecular Weight:	
Wt% < 500:	Wt% < 1000:
Physical State - Neat:	Solid
Melting Point:	Melting Point (est):
MP (EPI):	
Vapor Pressure:	Vapor Pressure (est):
VP (EPI):	<0.000001
Water Solubility:	Water Solubility (est):
Water Solubility (EPI):	>278
Henry's Law::	
Log Koc:	Log Koc (EPI):
Log Kow:	Log Kow (EPI):
Log Kow Comment:	

SAT**Concern Level**

Ecotox Rating (1):	3
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	All releases to water

Ecotox Comments

Exposure Based Review (Eco):
Ecotox Comments:
Exposure Based Testing:

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
1	1		Anion Ethanolamine

Persistence	Bioaccumulation	Toxicity	Comments
1	1		Anion Triethanolamine
3	*		Cation, B*(low)

Eco-Toxicity Comment:

Fate Ratings

Removal 75-90;50-90;75-90 Anion Ethanolamine;Anion in WWT/POTW Triethanolamine;Cation.							
(Overall): Condition	Rating Values	1	2	3	4	Rating Description Comment	
Fish BCF:							
Log Fish BCF:							
WWT/POTW Sorption:	1;1;3	Low	Moderate	Strong	V. Strong	Anion Ethanolamine;Anion Triethanolamine;Cation.	
WWT/POTW Stripping:	3;3;4	Extensive	Moderate	Low	Negligible	Anion Ethanolamine;Anion Triethanolamine;Cation.	
Biodegradation Removal:	2;2-3;4	Unknown	High	Moderate	Negligible	Anion Ethanolamine;Anion Triethanolamine;Cation.	
Biodegradation Destruction:		Unknown	Complete	Partial	—		
Aerobic Biodeg Ult:	2;2;4	<= Days	Weeks	Months	> Months	Anion Ethanolamine;Anion Triethanolamine;Cation.	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months		
Anaerobic Biodeg Ult:	2;2;4	<= Days	Weeks	Months	> Months	Anion Ethanolamine;Anion Triethanolamine;Cation.	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months		
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months		
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months		
Sorption to Soils/Sediments:	4;4;1	V. Strong	Strong	Moderate	Low	Anion Ethanolamine;Anion Triethanolamine;Cation.	
	3;3;1	Negligible	Slow	Moderate	Rapid		

Removal 75-90;50-90;75-90 Anion Ethanolamine;Anion in WWT/POTW Triethanolamine;Cation. (Overall):						
Condition	Rating Values	1	2	Rating Description 3	4	Comment
Migration to Ground Water:						Anion Ethanolamine;Anion Triethanolamine;Cation.
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	
Bio Comments:	Ethanolamine Anion Fish log BAF = -0.05 (1). Triethanolamine Anion Fish log BAF = -0.05 (1). The fugacity spreadsheets and the EPI output files for the ethanolamine and triethanolamine anions of the PMN material are attached.					
Fate Comments:						

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	0.9		Predictions are based on the standard toxicity profile for copper compounds with MW adj. (33% Cu).
Daphnid	48-h	LC50	0.078		Predictions are based on the standard toxicity profile for copper compounds with MW adj. (33% Cu).
Green Algae	96-h	EC50	0.11		Predictions are based on the standard toxicity profile for

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	-	Chronic Value	0.078		copper compounds with MW adj. (33% Cu). Predictions are based on the standard toxicity profile for copper compounds with MW adj. (33% Cu).
Daphnid	-	Chronic Value	0.051		Predictions are based on the standard toxicity profile for copper compounds with MW adj. (33% Cu).
Green Algae	-	Chronic Value	0.029		Predictions are based on the standard toxicity profile for copper compounds with MW adj. (33% Cu).
<p>Ecotox Value Predictions are based on the standard toxicity profile for copper compounds with MW adj. (33% Cu); MW 182; solid with unknown MP (P); S >278,000 mg/L (P); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO₃; and TOC <2.0 mg/L.</p> <p>Comments:</p>					

Ecotox Factors

Factors Most Sensitive Endpoint		Assessment Factor	CoC	Comment
Acute Aquatic (ppb):	78	5	16	The acute COC is based on the aquatic invertebrate EC50 toxicity value.
Chronic Aquatic(ppb):	29	10	3	The chronic COC is based on the algal ChV.

Factors	Values	Comments
SARs: SAR Class:		

Factors	Values	Comments
TSCA NCC Category?	None	

Recommended**Testing:****Ecotox Factors** Environmental

Comments: Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using hazard data on analogous chemicals. Acute toxicity values estimated for fish, aquatic invertebrates, and algae are 0.9 mg/L, 0.078 mg/L, and 0.11 mg/L, respectively. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are 0.078 mg/L, 0.051 mg/L, and 0.029 mg/L, respectively. These toxicity values indicate that the new chemical substance is expected to have high environmental hazard. Application of assessment factors of 5 and 10 to acute and chronic toxicity values, respectively, results in acute and chronic concentrations of concern of 0.016 mg/L (16 ppb) and 0.003 mg/L (3 ppb), respectively.

Environmental Risk: Risks to the environment were not identified due to no releases to water.

Comments/Telephone Log

Artifact	Update/Upload Time
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