TW 12/11/23
DSB 12/27/23
PT 04/15/24

Fate Report for Case # P-21-0126 (Version name 1)

Fate Summary Statement

Fate Summary Statement: P-21-0126
FATE: MW = 1849 with 6.59% < 500 and 16.84% < 1000
Solid
S = Disp.
VP < 1.0E-6 torr at 25 °C (E)
BP > 400 °C (E)
H < 1.00E-8 (E)
POTW removal (%) = Anion 95 via biodeg; Cation 90 via sorption
Time for complete ultimate aerobic biodeg = Anion wk; Cation > mo
Sorption to soils/sediments = Anion low; Cation v.strong
PBT Potential: Anion P1B1; Cation P3B1
FATE: Migration to ground water = Anion negl; Cation negl
Bioconcentration factor to be put into E-FAST: Anion N/A; Cation N/A

Analogue data found (include identifier and database)
Relevant Structure(s)
Water Parent
Landfill Parent
Air / Incineration Parent
Parent % incineration 99.9%

Environmental Fate Determination

PMN #: P-21-0126
Summary: EPA estimated that the anion 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 has low potential for bioaccumulation, such that 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 anion using data available for the anion and EPI (Estimation Program Interface) Suite™ (http://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface) and of the cation using data for analogue(s) (polymers). In wastewater treatment, the anion is expected to be removed with an efficiency of 95% due to biodegradation and the cation is expected to be removed with an efficiency of 90% due to sorption. Removal of the anion by biodegradation is high and removal of the cation by biodegradation is negligible. Sorption of the anion 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 anion to groundwater is expected to be negligible due to 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 anion is expected to undergo low volatilization to air and the cation is expected to undergo negligible volatilization due to low estimated vapor pressure and Henry's law constant. Overall, these estimates indicate that the anion and the cation have low potential to volatilize to air and low potential to 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 anion using data available for the anion and of the cation using data for analogue(s) (polymers). EPA estimated that the anion'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 anion 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 anion to bioaccumulate using data available for the anion and of the cation to bioaccumulate using data for analogue(s) (polymers). EPA estimated that the anion has low bioaccumulation potential based on high water solubility, which increases elimination and the cation has low bioaccumulation potential based on large predicted molecular volume, which limits bioavailability. EPA estimated that the anion 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 has low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

[redacted]

Fate Assessor: Tobias, David
SMILES: [redacted]

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	[redacted]	
Molecular Wt.:	1849.0	
% < 500:	6.59	
% < 1000:	16.84	

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:					
Boiling Point:					
BP Pressure:					
Vapor Pressure:			<0.000001		
Water Solubility:			Dispersible		
Log P:					
Log Kow:					

Property	Measured Value	Method	Estimated Value	Method	EPI
Log Koc:					
Log BCF:					
Henry's Law:					

pH:	
pH Comment:	

Fate Analysis

Hydrolysis (t1/2, da):	Volatilization (t1/2) - River (hr):	Volatilization (t1/2) - Lake (da):
Atm Ox Potential (t1/2)OH (hr):	Atm Ox Potential (t1/2)O3 (hr):	Atm Ox Potential(t1/2) Total (hr):
MITI Linear:	MITI NonLinear:	
Biodeg Linear:	Biodeg NonLinear:	
Biodeg Survey ult:	Biodeg Survey Prim:	
STP (% removal) Total:	STP (% removal) Biodeg:	
STP (% removal) Ads:	STP (% removal) Air:	

Rationales

Removal in Wastewater Treatment:	
Atmospheric Oxidation:	
Hydrolysis:	
Photolysis:	
Aerobic Biodegradation:	
Anaerobic Biodegradation:	
Sorption to Soil and Sediment:	
Migration to Groundwater:	
Persistence - Air:	
Persistence - Water:	
Volatilization from Water:	
Soil:	
Sediment:	
Other:	
Standard:	
Bioaccumulation:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
1	1		Anion
3	1		Cation

Exposure-Based Testing

Exposure-Based Testing:	

Fate Ratings

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	1;3	Low	Moderate	Strong	V. Strong	Anion;Cation
WWT/POTW Stripping:	3;4	Extensive	Moderate	Low	Negligible	Anion;Cation
Biodegradation Removal:	2;4	Unknown	High	Moderate	Negligible	Anion;Cation
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2;4	<= Days	Weeks	Months	> Months	Anion;Cation
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	2;4	<= Days	Weeks	Months	> Months	Anion;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;1	V. Strong	Strong	Moderate	Low	Anion;Cation
Migration to Ground Water:	1;1	Negligible	Slow	Moderate	Rapid	Anion;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	

Removal in WWT/POTW (Overall):	95;90 Anion;Cation
Bio Comments:	
Fate Comments:	

Comments/Telephone Log

Attachments	Update/Upload Time	Update/Upload By

Historic Documents

Attachments	Version Number	Updated/Uploaded Time	Updated/Uploaded By

Current Version Comments

Comment	Update/Upload Time	Update/Upload By