

Summary of Initial Risk Assessment Report

Acetonitrile CAS No : 75-05-8

PRTR No of Japan: 12

This substance is assessed based on Guideline for Initial Risk Assessment Version 1.0

1. General Information

1.1 Physico-chemical properties

Appearance	Colorless liquid
Melting point	-45 (degC)
Boiling point	81.6 (degC)
Water solubility	Miscible
Henry's constant	3.49 Pa*m ³ /mol (3.45*10 ⁻⁵ atm*m ³ /mol) (25degC, measured)
Octanol/water partition coefficient (log Kow)	-0.34 (measured), -0.15 (estimated)
Soil adsorption coefficient	Koc = 5 (estimated)

1.2 Environmental fate

Bioaccumulation	Low bioaccumulative Bioconcentration factor (BCF): 3.2 (calculated using logKow of -0.34)
Biodegradation	Readily biodegradable Considered to be biodegradable substance under aerobic and anaerobic conditions.

Stability in the environment	<p>(In air)</p> <p>Reaction with OH radical: Reaction rate constant is 2.63×10^{-14} cm³/molecule-sec. (25 degC, measured) The half - life is 0.8 - 2 years, given OH radical concentration of $5 \times 10^5 - 1 \times 10^6$ molecule/cm³.</p> <p>Reaction with ozone: Reaction rate constant is 1.50×10^{-19} cm³/molecule-sec. (25 degC, measured value) The half - life is 2 months, given ozone concentration of 7×10^{11} molecule/cm³.</p> <p>Reaction with nitrate radical: Reaction rate constant is less than 5.00×10^{-11} cm³/molecule/sec. (25 degC, measured) Since the half - life when the concentration of nitrate radical is estimated 2.4×10^8 molecule/cm³ (10 ppt) is calculated for 20 years or more, the reaction with nitrate radical in the troposphere atmosphere can be disregarded.</p> <p>Acetonitrile is not degraded directly by light because photoabsorption is limited to the far-ultraviolet region of the electromagnetic spectrum.</p> <p>(In water)</p> <p>The hydrolysis in aquatic environments can be disregarded, since the hydrolysis half-life is 150,000 years or more at pH 7.</p>
Environmental fate	If released into water, acetonitrile is expected to be removed mainly by volatilization and biodegradation.

2. Sources of release to the environment

2.1 Annual production, import, export and domestic supply in 2002 (ton/year)

Production	Import	Export	Domestic supply	Remarks
7,000	500 - 1,000	500 - 1,000	7,000	--

2.2 Uses

Raw material for agricultural chemicals, medical products, fragrances and dyes; extraction agent for antibiotics; solvent for HPLC, etc.; solvent for color film processing; reactive solvent, refinement solvent, organic electro bath for lithium batteries, etc.

2.3 Release from the industries within the scope of PRTR system (in 2001)

Release sources		Air (ton)	Waters (ton)	Soil (ton)	Remarks
Listed industries	Reported release	267	8	0	Release to rivers: 6.89 tons
	Release outside notification	15	<0.5	0	
Release outside notification from non listed industry		16	0	0	
Households		--	--	--	
Mobile sources		--	--	--	
Total		298	8	0	

2.4 Releases from other sources

It has been reported that acetonitrile is generated by incineration of wood, straw, and other plants.

2.5 Main release route

Acetonitrile is expected to be released into the environment mainly during use of the substance or products containing it.

3. Exposure Assessment

3.1 Measured environmental concentration

Media	No. of points detected / No. of points measured	No. of samples detected / No. of samples measured	Detection range	95th percentile	Detection limit	Year of investigation, Institution
Air (microg/m ³)	7/7	17/17	0.093-1.2	1.1	0.0008-0.076	2001 Ministry of the Environment
River water (microg/L)	0/44	--	nd	--	3	2000 Ministry of the Environment
Sea water	0/11	--	nd	--	3	2000 Ministry of the Environment
Drinking water (microg/L)(as ground water)	0/15	--	nd	--	3	2000 Ministry of the Environment
Food	--	--	--	--	--	--

nd: Not detected

For calculation of the 95th percentile, data less than the detection limit are replaced with a value equal to 1/2 of the detection limit.

3.2 Estimated environmental concentration

Media	Estimated concentration	Description
Air (microg/m ³)	0.554	Calculated by mathematical model / Atmospheric Dispersion Model for Exposure and Risk Assessment (AIST-ADMER) ver. 1.0
River water (microg/L)	14	Calculated by mathematical model / Initial Assessment System for the PRTR chemicals (IAS)

3.3 Estimated environmental concentration in water (EEC)

EEC(microg/L)	1.5
	The value (1.5microg/L) equal to 1/2 of detection limit was used for the risk assessment, since acetonitrile was not detected in any samples in the survey by the Ministry of the Environment in 2000 ¹⁾ .

3.4 Estimated human intake

Intake route		Concentration used for estimation of intake	Estimated intake (microg/person/day)	Estimated intake (microg/kg-Bodyweight (BW)/day)
Inhalation	Air	1.1 (microg/m ³)	22	0.44
		The 95 th percentile (1.12 microg/m ³) of measured concentrations surveyed by the Ministry of the Environment was used for the risk assessment.		
Oral	Drinking water	1.5 (microg/L)	3	0.06
		Measured concentrations in ground water were used, since measured concentrations in drinking water were not available. The value equal to 1/2 of detection limit was used for the risk assessment, since acetonitrile was not detected in any samples in the survey by the Ministry of the Environment.		
	Food	0.00474 (microg/g)	0.57	0.011
		-The concentration in fish was estimated as a product of concentration in sea water and BCF (3.16L/kg). -The value (1.5microg/L) equal to 1/2 of detection limit was used for concentration in seawater, since acetonitrile was not detected in any samples in the survey by the Ministry of the Environment in 2000.		
Subtotal		--	3.57	0.071
Total route		--	26	0.51

1) This substance is assessed based on the Guideline for Initial Risk Assessment Version1.0. If adequate measured concentrations are available, they are given priority and used as values for risk assessment. If they are not available, an estimated value calculated using a mathematical model is used.

4. Hazard assessment

4.1 Effects on organisms in the environment

	Acute or Chronic	Species	Endpoint	Concentration
Algae	Acute	<i>Lemna minor</i>	96 hours NOEC, Growth inhibition	1,000(mg/L)
Crustacea	Chronic	<i>Daphnia magna</i>	21 days NOEC Mortality of parents	300(mg/L)
Fish	Chronic	<i>Oryzias latipes</i>	21 days NOEC Mortality, Growth	102 or higher (mg/L)
Key study		Data of crustacea (<i>Daphnia magna</i>) was chosen for the key study because effects were observed at the lowest concentration in the hazard assessment.		

4.2 Human health toxicity

Toxicity	Exposure route	Species	Duration / Dose method	Toxic effects (Key study is underlined)	NOAEL or LOAEL (converted)
Repeated dose toxicity	Inhalation	Mouse	13 weeks	<u>Focal or multifocal discoloration, dark brown or black lesions of forestomach, epithelial hyperplasia of forestomach associated with focal ulcers in females,</u> hypoactivity, hunched and rigid posture, hepatocellular cytoplasmic vacuolation, increased absolute and relative liver weights, focal or multifocal squamous epithelial hyperplasia and focal ulcers of forestomach	NOAEL100ppm (168 mg/m ³) (equivalent to 50 mg/kg/day)
	Oral	--	--	--	--
	Dermal	--	--	--	--
	--	--	--	--	--
Carcinogenicity	Evaluation by IARC : This substance has not been evaluated by IARC				
Genotoxicity	Unable to determine genotoxicity				

5. Risk Assessment

5.1 Environmental organisms

Risk characterization	EEC (microg/L)	NOEC * (mg/L)	MOE (NOEC * /EEC)	Product of uncertainty factors	Conclusion
	1.5	NOEC: 300	200,000	50	No immediate concern
Product of uncertainty factors (UF): Extrapolation from laboratory test (10) * Toxicity data on two nutritional stages (5) = 50					
Recommendation : The substance is considered to be of no immediate concern for the moment, and low priority of further work.					

NOEC* means NOEC, LOEC, EC₅₀, etc.

5.2 Human health

5.2.1 Repeated dose toxicity

Exposure route	Intake (microg/kgBW/day)	NOAEL (mg/kgBW/day)	Risk characterization		
			MOE	Product of uncertainty factors	Conclusion
Inhalation	0.44	50	110,000	500	No immediate concern
Oral	0.071	No adequate data	Not calculated	Not calculated	Could not be assessed
Total	0.51	50 (Inhalation)	98,000	500	No immediate concern
Product of uncertainty factors (UF): Inhalation/Oral: Interspecies (10) * Intraspecies (10) * Duration of test (5) = 500					

5.2.2 Reproductive and developmental toxicity

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5.2.3 Carcinogenicity

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5.2.4. Recommendation for Human Health

In terms of inhalation exposure, the substance is considered to be of no immediate concern for the moment, and a low priority of further work. As for oral exposure, a risk assessment was not conducted because of no toxicity data.

6. Supplement

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