

ACETONITRILE
ECOLOGICAL FATE AND EFFECTS PROFILE

CAS No. 75 - 05 - 8

Prepared for

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Chemical Name: Acetonitrile

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1.0 SUMMARY

Acetonitrile is released to the environment during its manufacture and use from shale oil retorting and coal gasification, incineration of polyacrylonitrile from automobile exhaust and cigarette smoke.

Adsorption of acetonitrile to suspended solids and sediment in water and bioconcentration in aquatic organisms would not be important due to the high water solubility and low K_{OC} of acetonitrile. However, volatilization from dry and moist soil surface and leaching into groundwater would be important due to the value of Henry's Law constant, the moderately high vapor pressure (87 mm Hg 24°C) of acetonitrile and the high water solubility.

If released to soil, aerobic biodegradation is likely to occur. Acetonitrile is expected to be mobile in soil and may evaporate from soil surfaces.

Biodegradation is expected to be a major loss process in water. Acclimatization increases the biodegradation rate substantially. Volatilization may become competitive with other loss processes particularly at shallow water depth. Hydrolysis, photolysis, adsorption to suspended particles and sediments and bioconcentration in aquatic organisms are not likely to be important fate mechanism.

Acetonitrile is likely to be unreactive towards direct photolysis in air and the half-lives for its reaction with OH radicals and ozone have been estimated to be 535 days and 860 days, respectively. Therefore it will persist in the troposphere for a long time and may be transported long distance from its source of emission.

Acetonitrile is not expected to bioconcentrate in aquatic organisms due to low bioconcentrate factor. Acetonitrile is considered nontoxic to invertebrates, freshwater, algae and benthic organisms.

2.0 Environmental Fate

2.1 Environmental Fate Data

TYPE OF FATE	DATA	REFERENCE
Hydrolysis	first order 1195E-07	Brown et al., 1975
Water Solubility	miscible with water	Merck, 1989
Photolysis - soil	N.A. ¹	
Photolysis - water	Half-life = 676 days	Brown et al., 1975
Photolysis - air	half-life = 5501 years	Graedel, 1978
	Half-life = 535 - 860 days	Atkinson et al., 1984; Dimitruades et al., 1977
Sorption/desorption (K_d)	N.A.	
Organic Carbon/Water Partition Coefficient (K_{OC})	$K_{OC} = 16$	Lyman, 1982; Hansch and Leo, 1985
Octanol/water partition Coefficient (K_{OW})	$\text{Log } K_{OW} = -0.34$	Hansch and Leo, 1984
Bioconcentration - Bluegill Sunfish	$\text{Log } \text{BCF} = 0.87$	Neely et al., 1974
	$\text{BCF} = 0.3$	Lyman, 1982
Henry's Law Constant	$2.04 \times 10^{-5} \text{ atm m}^3/\text{mole}$	Snider and Dawson, 1985
	$3.46 \times 10^{-5} \text{ atm m}^3/\text{mole}$	Hine and Mookerjee, 1975
Vapor Pressure	79.9 mm Hg at 20°C	CHEMFATE, 1998
	87 mm Hg 24°C	Clayton and Clayton, 1981

¹ N.A. = not available

2.2 Summary of Environmental Fate of Acetonitrile

2.2.1 Environmental Degradation/Bioconcentration: Adsorption of acetonitrile to suspended solids and sediment in water and bioconcentration in aquatic organisms would not be important due to the high water solubility and low K_{OC} of acetonitrile. However, volatilization from dry and moist soil surface and leaching into groundwater would be important due to the value of Henry's Law constant, the moderately high vapor pressure (87 mm Hg 24°C) of acetonitrile and the high water solubility.

2.2.2 Aquatic Fate: A number of biodegradation studies with sewage activated sludge and pure cultures serving as microbial organisms have shown that acetonitrile is biodegradable in water following acclimatization as long as its original concentration is not too high (e.g. 500 mg/L) (Ludzack et al., 1958; Kagiya et al., 1975; Dimitriades et al., 1977). The decomposition of the compound (conc. 0.1 to 25 mg/L) in Ohio River water was 20% in 5 days and 40% in 12

days (Ellington et al., 1988). Biodegradation was faster in water following acclimatization. Photochemical studies in the vapor phase (Snider et al., 1985; Lyman et al., 1982) suggest that photodegradation in water may not be important. Hydrolysis is unimportant at the pH range normally present in natural waters (Ellington et al., 1988). Based on the value of 2.93×10^{-5} atm m^3/mole for Henry's Law Constant (Snider et al., 1985) and the relationship between Henry's Law constant and volatility (Lyman et al., 1982) of the compound from water may not be rapid, but may become competitive with other loss processes particularly at shallow water depths. The high water solubility and low K_{OC} of acetonitrile would suggest that adsorption of the compound to suspended solids and sediment in water and bioconcentration in aquatic organisms would not be important.

2.2.3 Atmospheric Fate: The rate constant for the reaction of acetonitrile with OH radicals in air has been determined to range from 1.9×10^{-14} to 4.94×10^{-14} $\text{cm}^3/\text{molecule-sec}$ in the temperature range 20-27°C (Atkinson, 1985; Wallington et al., 1988; Harris et al., 1981; Gusten et al., 1984; Gusten et al., 1981). Based on a rate constant of 3×10^{-14} $\text{cm}^3/\text{molecule-sec}$ and the average daily OH radicals concentration of 5×10^5 radicals/ cm^3 in the atmosphere (Atkinson, 1985), the half-life of this reaction is 535 days. The rate constant for the reaction of acetonitrile in air with ozone is 1.3×10^{-20} $\text{cm}^3/\text{molecule-sec}$ (Atkinson et al., 1984). In a typical atmosphere where the average daily ozone concentration is 7.2×10^{11} radicals/ cm^3 (Atkinson, 1985), the half-life due to this reaction would be 860 days. The photochemical smog studies also show that this compound is unreactive towards photochemically-generated free radicals (Dimitriades et al., 1977). Acetonitrile is also unreactive towards direct photolysis in the gas phase (Kagiya et al., 1975; Fujiki et al., 1978). In the atmosphere, acetonitrile is highly reactive to oxidizing materials (USEPA, 1980)

2.2.4 Terrestrial Fate: Photolysis studies in air (Kagiya et al., 1975; Dimitriades et al., 1977) and hydrolysis studies in water (Ellington et al., 1988) suggest that acetonitrile would not undergo appreciable photolysis or hydrolysis in soil. Based on an estimated K_{OC} value of 16 (Lyman, 1982; Hansch and Leo, 1985), acetonitrile would be weakly sorbed to most soils. The high water solubility, moderately high vapor pressure (Chiou et al., 1980) and weak soil sorption of the compound suggest that volatilization from soil surfaces and leaching into groundwater would be important.

2.2.5 Soil Adsorption and Soil Mobility: Based on a log K_{OW} value of -0.34 (Hansch and Leo, 1985) and a K_{OC} value of 16 (Lyman, 1982; Hansch and Leo, 1985), the sorption of acetonitrile onto soil or sediments will not be important.

2.2.6 Volatilization from Water and Soil: Based on a value of Henry's Law Constant of 2.93×10^{-5} atm m^3/mole (Snider et al., 1985), the volatilization half-life of acetonitrile from a 1 m deep river water flowing at a current speed of 1 m/sec and a wind speed of 3 m/sec would be 21 hours. Therefore, volatility of acetonitrile from water may become competitive with other loss processes, particularly at shallow water depths. The volatility of acetonitrile from soil has not been studied. The value of Henry's Law Constant and the moderately high vapor pressure

(87 mm Hg 24°C) of the compound (Clayton and Clayton, 1981) indicated that volatilization from dry and moist soil surface would be important.

3.0 ENVIRONMENTAL EFFECTS

3.1 Environmental Effects Data

TYPE OF EFFECTS	DATA	REFERENCE
Acute LC ₅₀ Fathead Minnow (<i>Pimephales promelas</i>)	LC ₅₀ = 1,000 mg/L, 96-hour	Henerson et al., 1961
	LC ₅₀ = 1,640 mg/L, 96-hour	Brooke et al., 1984
Acute LC ₅₀ Bluegill (<i>Lepomis macrochirus</i>)	LC ₅₀ = 1,850 mg/L, 96-hour	Verschueren, 1996
Acute LC ₅₀ Guppy (<i>Poeculia reticulata</i>)	LC ₅₀ = 1,650 mg/L, 96-hour	Henerson et al., 1961
Acute LC ₅₀ Gross Shrimp (<i>Palaemonetes kadiakensis</i>)	LC ₅₀ = 5,140 mg/L, 18-hour	Bowman et al., 1981
Acute LC ₅₀ <i>Daphnia magna</i>	LC ₅₀ = 10,000 mg/L, 24-hour	Bringmann et al., 1977
	LC ₅₀ = >10,000 mg/L, 96-hour	Ewell et al., 1986
Acute LC ₅₀ <i>Daphnia pulex</i>	LC ₅₀ = 5,810 mg/L, 18-hour	Bowman et al., 1981
Acute Toxicity - marine organisms - Shrimp (<i>Crangon crangon</i>)	N.A.	
Early Life Stage - Bluegill Sunfish (<i>Lepomis macrochirus</i>)	N.A.	
Chronic Life Cycle - Daphnia	N.A.	
Avian/Terrestrial wildlife oral LD ₅₀ Toxicity	N.A.	
Avian/Terrestrial Wildlife Dietary LC ₅₀ Toxicity	N.A.	
Chronic Avian/Terrestrial Wildlife Toxicity	N.A.	
Acute Toxicity - Green Algae (<i>Scenedesmus quadricauda</i>)	7,300 mg/L	Verschueren, 1996
Acute Toxicity - Algae (<i>Microcystis aeruginosa</i>)	520 mg/L	Verschueren, 1996
Bacteria - Toxicity Test	N.A.	
Acute Toxicity to Benthic organisms – Ramshorn snail (<i>Helisoma trivolvis</i>)	LC ₅₀ = >100 ug/L, 96-hour	Ewell et al., 1986

3.2 Summary of Environmental Effects of Acetonitrile

3.2.1 Acute Toxicity to Aquatic Organisms: The available information indicates that acetonitrile is considered non toxic to freshwater and invertebrate organisms.

3.2.2 Acute Toxicity to Benthic Organisms or Animals Exposed to Contaminated Sediments: Acetonitrile is not toxic to flatworm in an acute toxicity test.

3.2.3 Acute Toxicity to Terrestrial Wildlife via Oral Dose: No data available.

3.2.4 Acute Toxicity to Terrestrial Wildlife via Diet or Food: No data available.

3.2.5 Acute Toxicity to Plants or Soil Organisms Exposed through Soil Concentrations: No data available.

3.2.6 Chronic Toxicity to Aquatic Organisms: No data available.

3.2.7 Chronic Toxicity to Terrestrial Wildlife via Diet or Food: No data available.

3.2.8 Toxicity to Bacteria or Algae: No data available.

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5.0 SOURCE

Computer data base: April, 1998
HSDB (Hazardous Substances Databank)
BIODEG
CHEMFATE
DATALOG
AQUIRE

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