Material Safety Data Sheet

Acetonitrile, LC-MS



Section 1. Product and Company Identification

Product name : Acetonitrile, LC-MS

Product code : AX0156

Synonym: Ethanenitrile; Methyl Cyanide

Material uses : Other non-specified industry: Analytical reagent.

Manufacturer : EMD Chemicals Inc.

P.O. Box 70

480 Democrat Road Gibbstown, NJ 08027

856-423-6300 Technical Service Monday - Friday: 8:00 - 5:00 PM

Validation date : 4/1/2006.

Print date : 6/21/2006.

In case of emergency : 800-424-9300 CHEMTREC (USA)

613-996-6666 CANUTEC (Canada) 24 Hours/Day: 7 Days/Week

Section 2. Hazards Identification

Physical state : Liquid. (Colorless.)

Odor : Aromatic.

OSHA/HCS status : This material is considered hazardous by the OSHA Hazard Communication Standard

(29 CFR 1910.1200).

Emergency overview : DANGER! POISON!

HARMFUL IF INHALED, ABSORBED THROUGH SKIN OR SWALLOWED. CAUSES DAMAGE TO THE FOLLOWING ORGANS: KIDNEYS, LIVER,

CARDIOVASCULAR SYSTEM, RESPIRATORY TRACT, SKIN, CENTRAL NERVOUS

SYSTEM, EYE, LENS OR CORNEA. FLAMMABLE LIQUID AND VAPOR. VAPOR MAY CAUSE FLASH FIRE.

MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION.

BREATHING HIGH VAPOR CONCENTRATIONS MAY CAUSE CYANIDE POISONING. Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist.

Keep away from heat, sparks and flame. Keep container closed. Use only with

adequate ventilation. Wash thoroughly after handling.

Routes of entry : Dermal contact. Eye contact. Inhalation. Ingestion.

Potential acute health effects

Eyes: Moderately irritating to eyes.

Skin: Toxic in contact with skin. Moderately irritating to the skin.

Inhalation: Toxic by inhalation. Moderately irritating to the respiratory system.

Ingestion: Toxic if swallowed.

Carcinogenic effects
 Mutagenic effects
 No known significant effects or critical hazards.
 Teratogenicity /
 No known significant effects or critical hazards.
 No known significant effects or critical hazards.

Reproductive toxicity
Medical conditions

aggravated by over-

exposure

: Repeated skin exposure can produce local skin destruction or dermatitis. Repeated or

prolonged exposure to the substance can produce lung damage. Repeated or

prolonged contact with spray or mist may produce chronic eye irritation and severe skin irritation. Repeated or prolonged exposure to the substance can produce target organs

damage.

See toxicological information (section 11)

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Section 3. Composition/Information on Ingredients

United States

CAS number Name % by Weight Acetonitrile 75-05-8

Section 4. First Aid Measures

Eye contact : Get medical attention immediately. Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Check for and remove

any contact lenses.

Skin contact : Get medical attention immediately. Flush contaminated skin with plenty of water. Continue to rinse for at least 10 minutes. Remove contaminated clothing and shoes.

Wash contaminated clothing thoroughly with water before removing or wear gloves.

Wash clothing before reuse. Clean shoes thoroughly before reuse.

Inhalation : Get medical attention immediately. Move exposed person to fresh air. If it is suspected

that fumes are still present, the rescuer should wear an appropriate mask or selfcontained breathing apparatus. Keep person warm and at rest. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouthto-mouth resuscitation. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar,

tie, belt or waistband.

Ingestion : Get medical attention immediately. Wash out mouth with water. Remove dentures if

any. Move exposed person to fresh air. Keep person warm and at rest. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Stop if the exposed person feels sick as vomiting may be dangerous. Do not induce vomiting unless directed to do so by medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as

a collar, tie, belt or waistband.

Protection of first-aiders No action shall be taken involving any personal risk or without suitable training. If it is

suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to

give mouth-to-mouth resuscitation.

Section 5. Fire Fighting Measures

Flammability of the product: Flammable liquid and vapor. Vapor may cause flash fire. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash

back. Runoff to sewer may create fire or explosion hazard.

Products of combustion : These products are carbon oxides (CO, CO₂), nitrogen oxides (NO, NO₂ etc.).

Extinguishing media

Suitable : Use dry chemical, CO₂, water spray (fog) or foam.

Not suitable : Do not use water jet.

: Not available. Special exposure hazards

Special protective : Fire-fighters should wear appropriate protective equipment and self-contained breathing equipment for fire-fighters

apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Special remarks on fire : Dangerous fire and explosion risk. Vapor may travel a considerable distance to source hazards

of ignition and flash back.

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Section 6. Accidental Release Measures

Personal precautions

: Immediately contact emergency personnel. Eliminate all ignition sources. Keep unnecessary personnel away. Use suitable protective equipment. Do not touch or walk through spilled material.

Environmental precautions: Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Methods for cleaning up

: If emergency personnel are unavailable, contain spilled material. For small spills, add absorbent (soil may be used in the absence of other suitable materials) and use a nonsparking or explosion-proof means to transfer material to a sealable, appropriate container for disposal. For large spills, dike spilled material or otherwise contain material to ensure runoff does not reach a waterway. Place spilled material in an appropriate container for disposal.

Section 7. Handling and Storage

Handling

: Do not ingest. Avoid contact with eyes, skin and clothing. Keep container closed. Use only with adequate ventilation. Avoid breathing vapor or mist. Keep away from heat, sparks and flame. To avoid fire or explosion, dissipate static electricity during transfer by grounding and bonding containers and equipment before transferring material. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Wash thoroughly after handling.

Storage

Store in a segregated and approved area. Keep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid all possible sources of ignition (spark or flame).

Section 8. Exposure Controls/Personal Protection

Product name

United States

Acetonitrile

Exposure limits

ACGIH (United States, 1996).

STEL: 101 mg/m³ TWA: 67 mg/m³

OSHA (United States, 1989).

STEL: 105 mg/m³ TWA: 70 mg/m³

NIOSH REL (United States, 12/2001).

TWA: 34 mg/m³ 10 hour/hours. Form: All forms TWA: 20 ppm 10 hour/hours. Form: All forms

OSHA PEL (United States, 8/1997).

TWA: 70 mg/m³ 8 hour/hours. Form: All forms TWA: 40 ppm 8 hour/hours. Form: All forms OSHA PEL 1989 (United States, 3/1989).

STEL: 105 mg/m³ 15 minute/minutes. Form: All forms STEL: 60 ppm 15 minute/minutes. Form: All forms TWA: 70 mg/m³ 8 hour/hours. Form: All forms TWA: 40 ppm 8 hour/hours. Form: All forms

ACGIH TLV (United States, 1/2005). Skin Notes: Refers to Appendix A -- Carcinogens. 2002 Adoption.

TWA: 20 ppm 8 hour/hours. Form: All forms

Consult local authorities for acceptable exposure limits.

Engineering measures

: Use only with adequate ventilation. If user operations generate dust, fumes, vapor or mist, use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Personal protection

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Section 8. Exposure Controls/Personal Protection

Safety eyewear complying with an approved standard should be used when a risk

assessment indicates this is necessary to avoid exposure to liquid splashes, mists,

gases or dusts.

Recommended: splash goggles

: Personal protective equipment for the body should be selected based on the task being Skin

performed and the risks involved and should be approved by a specialist before handling

this product.

Body: Recommended: lab coat

: Use a properly fitted, air-purifying or air-fed respirator complying with an approved Respiratory

> standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe

working limits of the selected respirator.

Chemical-resistant, impervious gloves complying with an approved standard should be Hands

worn at all times when handling chemical products if a risk assessment indicates this is

necessary. Recommended: nitrile rubber

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before

eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash

contaminated clothing before reusing. Ensure that eyewash stations and safety showers

are close to the workstation location.

Section 9. Physical and Chemical Properties

Physical state : Liquid. (Colorless.)

: Closed cup: 5.85°C (42.5°F). Flash point

Auto-ignition temperature : 524°C (975.2°F)

Flammable limits : Lower: 3% Upper: 16%

Color : Colorless. Odor : Aromatic. Molecular weight : 41.06 g/mole Molecular formula : C2-H3-N

Boiling/condensation point: 81.67°C (179°F) **Melting/freezing point** : -41.9°C (-43.4°F) Critical temperature : 274.8°C (526.6°F) Relative density 0.787 (Water = 1)

Vapor pressure : 9.7 kPa (72.8 mm Hg) (at 20°C)

Vapor density : 1.42 (Air = 1)**Volatility** : 100% (v/v) **Odor threshold**

: 40 ppm

Evaporation rate : 2.33 compared with Butyl acetate.

VOC : 100 (%)

Section 10. Stability and Reactivity

Stability and reactivity : The product is stable.

Incompatibility with various: Highly reactive or incompatible with the following materials: oxidizing materials, reducing

materials, acids and alkalis.

Hazardous decomposition : carbon oxides (CO, CO₂) nitrogen oxides (NO, NO₂ etc.) Hydrogen cyanide (HCN).

products

substances

Hazardous polymerization : Will not occur. Acetonitrile, LC-MS AX0156 Page: 5/8

Section 10. Stability and Reactivity

Conditions of reactivity

: Highly flammable in the presence of the following materials or conditions: open flames, sparks and static discharge, heat, shocks and mechanical impacts and oxidizing

Dangerous fire and explosion risk. Vapor may travel a considerable distance to source of ignition and flash back.

Highly explosive in the presence of the following materials or conditions: open flames, sparks and static discharge, heat, shocks and mechanical impacts and oxidizing

Section 11. Toxicological Information

Toxicity data

United States

Product/ingredient name	<u>Test</u>	<u>Result</u>	<u>Route</u>	<u>Species</u>
Acetonitrile	LD50	2460 mg/kg	Oral	Rat
	LD50	50 mg/kg	Oral	Rabbit
	LD50	177 mg/kg	Oral	Guinea pig

Chronic effects on humans : CARCINOGENIC EFFECTS A4 (Not classifiable for humans or animals.) by ACGIH. Causes damage to the following organs: kidneys, liver, cardiovascular system, upper respiratory tract, skin, central nervous system (CNS), eye, lens or cornea.

Other toxic effects on

humans

: Very hazardous in case of skin contact (permeator), of ingestion, .

Hazardous in case of skin contact (irritant), of eye contact (irritant), of inhalation (lung

irritant).

Specific effects

Carcinogenic effects Mutagenic effects Teratogenicity / Reproductive toxicity : No known significant effects or critical hazards. : No known significant effects or critical hazards.

: No known significant effects or critical hazards.

Sensitization

Ingestion : No known significant effects or critical hazards. : Moderately irritating to the respiratory system. Inhalation

Eves : Moderately irritating to eyes. Skin : Moderately irritating to the skin.

Section 12. Ecological Information

Ecotoxicity data

United States

Product/ingredient name **Species** Period Result Acetonitrile Daphnia magna (LC50) >100 mg/l 96 hour/hours Pimephales promelas (LC50) 96 hour/hours >100 mg/l Pimephales promelas (LC50) 96 hour/hours 1640 mg/l

Environmental precautions: No known significant effects or critical hazards.

Products of degradation

: These products are carbon oxides (CO, CO₂) and water, nitrogen oxides (NO, NO₂ etc.).

Toxicity of the products of

biodegradation

: The products of degradation are less toxic than the product itself.

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Section 13. Disposal Considerations

Waste disposal

: The generation of waste should be avoided or minimized wherever possible. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements.

Disposal should be in accordance with applicable regional, national and local laws and regulations. Local regulations may be more stringent than regional or national requirements.

The information presented below only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations.

Refer to Section 7: HANDLING AND STORAGE and Section 8: EXPOSURE CONTROLS/PERSONAL PROTECTION for additional handling information and protection of employees.

Section 14. Transport Information

Regulatory information	UN number	Proper shipping name	Class	PG*	Label	Additional information
DOT Classification	UN1648	ACETONITRILE	3	II		Reportable quantity 5000 lbs. (2268 kg)

PG*: Packing group

Section 15. Regulatory Information

United States

HCS Classification : Flammable liquid

> Toxic material Irritating material Target organ effects

U.S. Federal regulations : TSCA 8(b) inventory: Listed

> SARA 302/304/311/312 extremely hazardous substances: No products were found. SARA 302/304 emergency planning and notification: No products were found.

SARA 302/304/311/312 hazardous chemicals: Acetonitrile

SARA 311/312 MSDS distribution - chemical inventory - hazard identification: Acetonitrile

: Fire hazard, Immediate (acute) health hazard, Delayed (chronic) health hazard

Clean Water Act (CWA) 307: Acetonitrile

Clean Water Act (CWA) 311: No products were found.

Clean Air Act (CAA) 112 accidental release prevention: No products were found. Clean Air Act (CAA) 112 regulated flammable substances: No products were found.

Clean Air Act (CAA) 112 regulated toxic substances: No products were found.

SARA 313

Product name

CAS number Concentration

Form R - Reporting

requirements

: Acetonitrile 75-05-8 100

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Section 15. Regulatory Information

Supplier notification: Acetonitrile 75-05-8 100

SARA 313 notifications must not be detached from the MSDS and any copying and redistribution of the MSDS shall include copying and redistribution of the notice attached to copies of the MSDS subsequently redistributed.

State regulations : Pennsylvania RTK: Acetonitrile : (environmental hazard, generic environmental hazard)

Massachusetts RTK: Acetonitrile

New Jersey: Acetonitrile

Canada

WHMIS (Canada) : Class B-2: Flammable liquid

Class D-1A: Material causing immediate and serious toxic effects (Very toxic).

Class D-2B: Material causing other toxic effects (Toxic).

CEPA DSL/CEPA NDSL : CEPA DSL: Acetonitrile

This product has been classified according to the hazard criteria of the CPR and the MSDS contains all the information required by the CPR.

EU regulations

Hazard symbol/symbols

Risk phrases : R11- Highly flammable.

R20/21/22- Harmful by inhalation, in contact with skin and if swallowed.

R36- Irritating to eyes.

Safety phrases : S1/2- Keep locked up and out of the reach of children.

S16- Keep away from sources of ignition - No smoking. S36/37- Wear suitable protective clothing and gloves.

International regulations

International lists : Australia (NICNAS): Acetonitrile

China: Acetonitrile

Germany water class: Acetonitrile

Japan (METI): Acetonitrile

Korea (TCCL): Acetonitrile

Philippines (RA6969): Acetonitrile

Section 16. Other Information

Label requirements : DANGER! POISON!

HARMFUL IF INHALED, ABSORBED THROUGH SKIN OR SWALLOWED. CAUSES DAMAGE TO THE FOLLOWING ORGANS: KIDNEYS, LIVER,

CARDIOVASCULAR SYSTEM, RESPIRATORY TRACT, SKIN, CENTRAL NERVOUS

SYSTEM, EYE, LENS OR CORNEA. FLAMMABLE LIQUID AND VAPOR. VAPOR MAY CAUSE FLASH FIRE.

MAY CAUSE RESPIRATORY TRACT, EYE AND SKIN IRRITATION.

BREATHING HIGH VAPOR CONCENTRATIONS MAY CAUSE CYANIDE POISONING.

National Fire Protection Association (U.S.A.)

Health 2 0 Instability
Special

Notice to reader

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Section 16. Other Information

The statements contained herein are based upon technical data that EMD Chemicals Inc. believes to be reliable, are offered for information purposes only and as a guide to the appropriate precautionary and emergency handling of the material by a properly trained person having the necessary technical skills. Users should consider these data only as a supplement to other information gathered by them and must make independent determinations of suitability and completeness of information from all sources to assure proper use, storage and disposal of these materials and the safety and health of employees and customers and the protection of the environment. EMD CHEMICALS INC. MAKES NO REPRESENTATION OR WARRANTY OF ANY KIND, EXPRESS OR IMPLIED, INCLUDING MERCHANTABILITY OR FITNESS FOR A PARTICULAR USE, WITH RESPECT TO THE INFORMATION HEREIN OR THE PRODUCT TO WHICH THE INFORMATION REFERS.