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SAFETY DATA SHEETS

According to the UN GHS revision 10

Version: 1.1
Creation Date: July 15, 2024
Revision Date: January 08, 2025

SECTION 1: Identification

1.1 GHS Product identifier

Product name 4 Stable Isotope Labeled Toxin Mix Solution in Acetonitrile, 0.5µg/mL

1.2 Other means of identification

Product number MCFD202428
Other names -

1.3 Recommended use of the chemical and restrictions on use

Identified uses For laboratory and Industrial use only.
Uses advised against no data available

1.4 Supplier's details

Company CATO Research Chemicals Inc.
Address 3/F,Building B,No.179 BASIGO, Guangpu Rd East,Huangpu Dist,Guangzhou
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1.5 Emergency phone number

Emergency phone number +86-20-81960175
Service hours 'Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Flammable liquids, Category 2
Acute toxicity - Category 4, Oral
Acute toxicity - Category 4, Dermal
Eye irritation, Category 2
Acute toxicity - Category 4, Inhalation

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word Danger
Hazard statement(s)
H225 Highly flammable liquid and vapour
H302 Harmful if swallowed
H312 Harmful in contact with skin
H319 Causes serious eye irritation
H332 Harmful if inhaled

Precautionary statement(s)
Prevention
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.

Response	P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower]. P370+P378 In case of fire: Use ... to extinguish. P301+P317 IF SWALLOWED: Get medical help. P330 Rinse mouth. P302+P352 IF ON SKIN: Wash with plenty of water/... P317 Get medical help. P321 Specific treatment (see ... on this label). P362+P364 Take off contaminated clothing and wash it before reuse. P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
Storage	P403+P235 Store in a well-ventilated place. Keep cool.
Disposal	P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Acetonitrile	Acetonitrile	75-05-8	200-835-2	≈ 99%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed. No mouth-to-mouth artificial respiration. Refer immediately for medical attention. See Notes.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

Rinse with plenty of water (remove contact lenses if easily possible). Refer immediately for medical attention.

Following ingestion

Rinse mouth. Give one or two glasses of water to drink. Do NOT induce vomiting. Refer immediately for medical attention.

4.2 Most important symptoms/effects, acute and delayed

Exposure to 160 ppm for 4 hours causes flushing of the face and a feeling of constriction in the chest; 500 ppm for brief periods is irritating to the nose and throat. Severe exposures cause irritability, skin eruptions, confusion, delirium, convulsions, paralysis, and death due to central nervous system depression. (USCG, 1999)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bog-valve-mask device, or pocket mask, as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Cyanide and related compounds

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Foam, carbon dioxide, dry chemical

5.2 Specific hazards arising from the chemical

Special Hazards of Combustion Products: Toxic vapors are generated when heated Behavior in Fire: Vapor heavier than air and may travel a considerable distance to a source of ignition and flash back. (USCG, 1999)

5.3 Special protective actions for fire-fighters

Use powder, foam, carbon dioxide. Water may be ineffective. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Consult an expert! Personal protection: complete protective clothing including self-contained breathing apparatus. Ventilation. Remove all

ignition sources. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in dry sand or inert absorbent. Then store and dispose of according to local regulations.

6.2 Environmental precautions

Consult an expert! Personal protection: complete protective clothing including self-contained breathing apparatus. Ventilation. Remove all ignition sources. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in dry sand or inert absorbent. Then store and dispose of according to local regulations.

6.3 Methods and materials for containment and cleaning up

ACCIDENTAL RELEASE MEASURES. Personal precautions, protective equipment and emergency procedures: Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.; Environmental precautions: Prevent further leakage or spillage if safe to do so. Do not let product enter drains.; Methods and materials for containment and cleaning up: Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames, NO sparks and NO smoking. NO contact with hot surfaces or strong oxidizing agents. Closed system, ventilation, explosion-proof electrical equipment and lighting. Do NOT use compressed air for filling, discharging, or handling. Use non-sparking handtools. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Fireproof. Keep in a well-ventilated room. Separated from acids, bases, strong oxidants and food and feedstuffs. Well closed.Protect containers against physical damage. Outdoor or detached storage is preferable. Separate from any sources of ignition and combustible materials. Storage room should be well-ventilated.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

TLV: 20 ppm as TWA; (skin); A4 (not classifiable as a human carcinogen).MAK: 17 mg/m3, 10 ppm; peak limitation category: II(2); skin absorption (H); pregnancy risk group: C.EU-OEL: 70 mg/m3, 40 ppm as TWA; (skin)

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear face shield or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Liquid.
Colour	Clear, colorless.
Odour	Aromatic odor
Melting point/freezing point	-45.7 °C.
Boiling point or initial boiling point and boiling range	81.6 °C. Atm. press.:1 013.25 hPa.
Flammability	Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F.
Lower and upper explosion limit/flammability limit	Lower flammable limit: 3.0%; Upper flammable limit: 16.0%
Flash point	12.8 °C.
Auto-ignition temperature	524 °C.
Decomposition temperature	no data available

pH	no data available
Kinematic viscosity	0.35 cP at 20 deg C
Solubility	Miscible with water
Partition coefficient n-octanol/water	log Pow = -0.34.
Vapour pressure	94.51 hPa. Temperature:20 °C. Remarks:Upper value: 98.64 hPa.
Density and/or relative density	0.79. Temperature:20 °C.
Relative vapour density	1.41 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Decomposes on heating or on burning and on contact with hot surfaces. This produces toxic fumes including hydrogen cyanide and nitrogen oxides. Reacts violently with strong oxidants. This generates fire and explosion hazard. Reacts with acids and bases. This produces toxic and flammable hydrogen cyanide. Attacks some forms of plastic, rubber and coatings.

10.2 Chemical stability

Heat /contributes to instability/.

10.3 Possibility of hazardous reactions

Dangerous fire hazard when exposed to heat, flame or oxidizers.The vapour mixes well with air, explosive mixtures are easily formed.ACETONITRILE decomposes when heated to produce deadly toxic hydrogen cyanide gas and oxides of nitrogen. Strongly reactive [Hawley]. May react vigorously with strong oxidizing reagents, sulfuric acid, chlorosulfonic acid, sulfur trioxide, perchlorates, nitrating reagents, and nitric acid. [Sax, 9th ed., 1996, p. 20]. Potentially explosive in contact with nitrogen-fluorine compounds (e.g., tetrafluorourea) [Fraser, G. W. et al., Chem. Comm., 1966, p. 532].

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

Strong oxidizers such as chlorine, bromine, and fluorine; chlorosulfonic acid; oleum or sulfuric acid. May accumulate static electricial charges, and may cause ignition of its vapors.

10.6 Hazardous decomposition products

When heated to decomposition, emits highly toxic fumes of /cyanides and nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - mouse (male) - 469 mg/kg bw.
- Inhalation: LC50 - mouse (male/female) - 3 587 ppm.
- Dermal: LD50 - rabbit (male/female) - > 2 000 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

Weight-of-Evidence Characterization Under the current Risk Assessment Guidelines (US EPA, 1987), ACN is assigned carcinogen class D, not classifiable as to human carcinogenicity. There is an absence of human evidence and the animal evidence is equivocal. Under the Proposed Guidelines for Carcinogen Risk Assessment (US EPA, 1996), the carcinogenic potential of ACN following inhalation, oral, or dermal exposure is best characterized as "cannot be determined because the existing evidence is composed of conflicting data (e.g., some evidence is suggestive of carcinogenic effects, but other equally pertinent evidence does not confirm any concern)." Based on former classification guidelines

Reproductive toxicity

No information is available on the reproductive or developmental effects of acetonitrile in humans. (1-3) Animal studies appear to suggest that acetonitrile may cause developmental and reproductive effects such as a decrease in average fetal body weight and a significant increase in the number of malformed offspring. (1-3)

STOT-single exposure

The substance is irritating to the eyes. The substance may cause effects on the cellular respiration (inhibition). This may result in convulsions and respiratory failure. Exposure far above the OEL could cause death. The effects may be delayed. Medical observation is

indicated.

STOT-repeated exposure

The substance may have effects on the blood. This may result in anaemia. The substance may have effects on the kidneys, liver and thyroid. This may result in impaired functions.

Aspiration hazard

A harmful contamination of the air can be reached rather quickly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 - Pimephales promelas - 1 640 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: LC50 - Artemia salina - 641 mg/L - 24 h.
- Toxicity to algae: EC50 - Phaeodactylum tricornutum - 3 560 mg/L - 72 h.
- Toxicity to microorganisms: EC50 - activated sludge - > 1 000 mg l-1 - 30 min.

12.2 Persistence and degradability

AEROBIC: Enzyme-catalyzed hydrolysis of nitriles, such as acetonitrile, has been shown to proceed by two distinct routes(1,2); a nitrilase transforms the nitriles directly into acids plus ammonium ion, or a nitrile hydratase forms the amide which is hydrolyzed to acid plus ammonium ion by amidase(1,2). A mixed microbial culture isolated from an environment contaminated with organic cyanides and PCBs utilized acetonitrile as the sole source of carbon and nitrogen(3). The mixed microbial culture was grown for 48 hrs at pH 7 with 1 g/L of acetonitrile; the final pH and ammonia concentration were determined to be 8.81 and 80.1 umol/mL, respectively(3). The biodegradation studies of acetonitrile with mixed cultures of microorganisms from activated sludge and sewage show that degradation proceeds sluggishly without acclimatization of microorganisms, particularly at high concentration(4,5). Degradation is faster with acclimatization(6-11). With activated sludge as microbial inoculum, the lag period of acetonitrile degradation was about 1 day after which the compound degraded with a half-life of 1.2 days(8). Acclimated mixed microbial cultures isolated by an enrichment culture technique degraded 58% acetonitrile in 5 days(9). The biodegradability of acetonitrile was also observed with river water; the 12 day ThOD (theoretical oxygen demand) with river water was 40%(10,11). Acclimation of the microorganisms was examined by redosing; the degradation was 5 times faster after acclimation; it was also 4 times faster at 20 deg C than at 5 deg C(10,11). The biodegradation is expected to be much slower in seawater than in freshwater(12). Acetonitrile, present at 100 mg/L, reached 65% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test which classified the compound as readily biodegradable(13).

12.3 Bioaccumulative potential

An estimated BCF of 3 was calculated in fish for acetonitrile(SRC), using a log Kow of -0.34(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

12.4 Mobility in soil

Acetonitrile has a reported measured Koc Value of 2.2(1). According to a classification scheme(2), this Koc value suggests that acetonitrile is expected to have very high mobility in soil(SRC).

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN1648 (For reference only, please check.)	IMDG: UN1648 (For reference only, please check.)	IATA: UN1648 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: ACETONITRILE (For reference only, please check.)	IMDG: ACETONITRILE (For reference only, please check.)	IATA: ACETONITRILE (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 3 (For reference only, please check.)	IMDG: 3 (For reference only, please check.)	IATA: 3 (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: II (For reference only, please check.) IMDG: II (For reference only, please check.) IATA: II (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: No IMDG: No IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
Acetonitrile	Acetonitrile	75-05-8	200-835-2
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

SECTION 16: Other information

Information on revision

Creation Date July 15, 2024
Revision Date January 08, 2025

Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home
- HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm
- IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple
- ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg
- Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp
- ECHA - European Chemicals Agency, website: https://echa.europa.eu/

Other Information

Specific treatment is necessary in case of poisoning with this substance; the appropriate means with instructions must be available.Oxygen should be administered exclusively by specially trained first aid or medical personnel.Do NOT take working clothes home.

Any questions regarding this SDS, Please send your inquiry to info@cato-chem.com

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