

Chemical Safety Data Sheet MSDS / SDS

Boron trifluoride acetonitrile complex

Revision Date:2026-05-31 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking**Product identifier**

Product name : Boron trifluoride acetonitrile complex
CBnumber : CB4497282
CAS : 420-16-6
EINECS Number : 690-796-1
Synonyms : Boron trifluoride acetonitrile complex

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification**GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

Precautionary statements

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H225 Highly Flammable liquid and vapour

H314 Causes severe skin burns and eye damage

H331 Toxic if inhaled

SECTION 3: Composition/information on ingredients

Substance

Product name	: Boron trifluoride acetonitrile complex
Synonyms	: Boron trifluoride acetonitrile complex
CAS	: 420-16-6
EC number	: 690-796-1
MF	: C ₂ H ₃ BF ₃ N
MW	: 108.86

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Hydrofluoric (HF) acid burns require immediate and specialized first aid and medical treatment. Symptoms may be delayed up to 24 hours depending on the concentration of

HF. After decontamination with water, further damage can occur due to penetration/absorption of the fluoride ion. Treatment should be directed toward binding the fluoride ion as well as the effects of exposure. Skin exposures can be treated with a 2.5% calcium gluconate gel repeated until burning ceases. More serious skin exposures may require subcutaneous calcium gluconate except for digital areas unless the physician is experienced in this technique, due to the potential for tissue injury from increased pressure. Absorption can readily occur through the subungual areas and should be considered when undergoing decontamination. Prevention of absorption of the fluoride ion in cases of ingestion can be obtained by giving milk, chewable calcium carbonate tablets or

Milk of Magnesia to conscious victims. Conditions such as hypocalcemia, hypomagnesemia and cardiac arrhythmias should be monitored for, since they can occur after exposure. First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

In case of skin contact

First treatment with calcium gluconate paste. In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

4.4 Notes to physician

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

Water Foam

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO_x)

Hydrogen fluoride

Borane/boron oxides

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

May not get in touch with: Water

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-

absorbent material (e.g.

Chemizorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Keep workplace dry. Do not allow product to come into contact with water.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition. Keep locked up or in an area accessible only to qualified or authorized persons.

Never allow product to get in contact with water during storage.

Storage stability Recommended storage temperature

2 - 8 °C

Do not store in glass

Storage class

Storage class (TRGS 510): 3: Flammable liquids

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

['Component', 'CAS-No.', 'Value', 'Control parameters', 'Basis']	['Acetonitrile', '75-05-8', 'PC-TWA', '30 mg/m3', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.']	['', 'Remarks', 'Skin', 'None', 'None']	['Boron Trifluoride', '7637-07-2', 'MAC', '3 mg/m3', 'Occupational exposure limits for hazardous agents in the workplace - Chemical hazardous agents.']
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Biological occupational exposure limits

['Component', 'CAS-No.', 'Parameters', 'Value', 'Biological']	
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specimen', 'Basis']						
['', 'Remarks', 'After shift', None, None, None]	['', '', 'fluoride', '7mg/g creatinin e', 'Urine', 'China. Biological Occupational Exposure Indices']	['', '', 'After shift', None, None, None]	['', '', 'fluoride', '24Millimoles per mole creatinin e', 'Urine', 'China. Biological Occupational Exposure Indices']	['', '', 'Prior to shift', None, None, None]	['', '', 'fluoride', '4mg/g creatinin e', 'Urine', 'China. Biological Occupational Exposure Indices']	['', '', 'Prior to shift', None, None, None]

7637-07-2 fluoride 42Millimoles Urine China. Biological moles per Occupational mole Exposure Indices creatinin e

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M) data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

a) Physical state	liquid
b) Color	Clear
c) Odor	No data available
d) Melting point/freezing point	No data available
e) Initial boiling point and boiling range	85.5 °C at 101.325kPa
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	3-17% (v/v) Information refers to the main component.)
h) Flash point	10 °C
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	No data available
l) Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
m) Water solubility	No data available
n) Partition coefficient n-octanol/water	No data available
o) Vapor pressure	84.1-301.3hPa at 20-50 °C
p) Density	0.87-0.88 g/mL at 20 °C
Relative density	0.87-0.88 g/mL at 20 °C
q) Relative vapor density	No data available
r) Particle characteristics	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Chemical stability

sensitive to moisture

10.2 Possibility of hazardous reactions

No data available

10.3 Conditions to avoid

Reacts dangerously with glass.

Warming.

Moisture.

10.4 Incompatible materials

glass

10.5 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture Acute toxicity

Oral: Harmful if swallowed.

Oral: No data available

Acute toxicity estimate Oral - 771.25 mg/kg (Calculation method)

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Acute toxicity estimate Inhalation - 4 h - 4.2 mg/l - vapor(Calculation method)

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Acute toxicity estimate Dermal - 1,875 mg/kg (Calculation method)

Skin corrosion/irritation

Remarks: Causes skin burns.

Remarks: Mixture causes burns.

Serious eye damage/eye irritation

Remarks: No data available

Remarks: Mixture causes serious eye damage.

Risk of blindness!

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components Acetonitrile

Acute toxicity

LD50 Oral - Mouse - male and female - 617 mg/kg (OECD Test Guideline 401)

LC50 Inhalation - Mouse - male and female - 4 h - 6.022 mg/l - vapor (OECD Test Guideline 403)

Acute toxicity estimate Dermal - 1,500 mg/kg (Expert judgment)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(OECD Test Guideline 405)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative (OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Result: negative

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Result: Positive results were obtained in some in vitro tests.

Remarks: (National Toxicology Program)

Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Result: negative

Remarks: Sister chromatid exchange

Test system: *Saccharomyces cerevisiae*

Result: positive

Remarks: Cytogenetic analysis (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female

Result: negative

Carcinogenicity

No evidence of carcinogenicity in animal studies.

Reproductive toxicity

Animal testing did not show any effects on fertility.

Specific target organ toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

No aspiration toxicity classification

Boron Trifluoride Acute toxicity

Oral: No data available

LC50 Inhalation - Rat - male and female - 4 h - 1.21 mg/l - vapor (OECD Test Guideline 403)

Dermal: No data available

Skin corrosion/irritation

Classified based on available data. For more details, see section 2

Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

Germ cell mutagenicity

Classified based on available data. For more details, see section 2

Carcinogenicity

Classified based on available data. For more details, see section 2

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Additional Remarks: No data available

Information

Components Acetonitrile

Toxicity to fish flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,640 mg/l - 96 h

Remarks: (ECHA)

Toxicity to algae static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (ISO 10253) static test ErC50 - Phaeodactylum tricornutum - 9,696 mg/l - 72 h (ISO 10253)

Toxicity to bacteria

Toxicity to flow-through test NOEC - Oryzias latipes - 102 mg/l - 21 d fish(Chronic toxicity) (OECD Test Guideline 204)

Boron Trifluoride

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 3286

IMDG: 3286

IATA-DGR: 3286

14.2 UN proper shipping name

ADR/RID: FLAMMABLE LIQUID, TOXIC, CORROSIVE, N.O.S. (Acetonitrile, Boron Trifluoride)

IMDG: FLAMMABLE LIQUID, TOXIC, CORROSIVE, N.O.S. (Acetonitrile, Boron Trifluoride)

IATA-DGR: Flammable liquid, toxic, corrosive, n.o.s. (Acetonitrile, Boron Trifluoride)

14.3 Transport hazard class(es)

ADR/RID: 3 (6.1, 8)

IMDG: 3 (6.1, 8)

IATA-DGR: 3 (6.1)(8)

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA-DGR: II

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

14.6 Special precautions for user

Based on chemical properties, choose appropriate tools and conditions of transport.

Transporting tools shall be equipped with appropriate and sufficient firefighting equipment and emergency leaking installations. If transporting by road, please go along the specified route.

14.7 Incompatible materials

glass

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulatory information

Law on the Prevention and Control of Occupational Diseases

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals : Listed

Other regulations

Please pay attention on the waste treatment should also comply with local regulations requirement.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

TWA: Time-Weighted Average

STEL: Short-Term Exposure Limit

LD50: Lethal Dose 50%

LC50: Lethal Concentration 50%

EC50: Effective Concentration 50%

PEL: Permissible Exposure Limit

TLV: Threshold Limit Value

IMDG: International Maritime Dangerous Goods Code

IATA: International Air Transport Association

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

DOT: US Department of Transportation

NFPA: National Fire Protection Association

NIOSH: National Institute for Occupational Safety and Health

OSHA: Occupational Safety and Health Administration

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.