

SAFETY DATA SHEET

Version 8.4
Revision Date 04/20/2021
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : 4-Cyanophenylzinc bromide solution

Product Number : 520292
Brand : Aldrich
CAS-No. : 131379-14-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 2), H225
Chemicals which, in contact with water, emit flammable gases (Category 2), H261
Acute toxicity, Oral (Category 4), H302
Eye irritation (Category 2A), H319
Carcinogenicity (Category 2), H351
Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, H336

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word	Danger
Hazard statement(s)	
H225	Highly flammable liquid and vapor.
H261	In contact with water releases flammable gas.
H302	Harmful if swallowed.
H319	Causes serious eye irritation.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
H351	Suspected of causing cancer.
Precautionary statement(s)	
P201	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P223	Do not allow contact with water.
P231 + P232	Handle under inert gas. Protect from moisture.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P308 + P313	IF exposed or concerned: Get medical advice/ attention.
P335 + P334	Brush off loose particles from skin. Immerse in cool water/ wrap in wet bandages.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P402 + P404	Store in a dry place. Store in a closed container.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

In use may form flammable/explosive vapor-air mixture., May form explosive peroxides.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Formula : C₇H₄BrNZn
Molecular weight : 247.41 g/mol

Component		Classification	Concentration
Tetrahydrofuran			
CAS-No.	109-99-9	Flam. Liq. 2; Acute Tox. 4;	>= 90 - <= 100 %
EC-No.	203-726-8	Eye Irrit. 2A; Carc. 2;	
Index-No.	603-025-00-0	STOT SE 3; H225, H302,	
Registration	01-2119444314-46-	H319, H351, H335, H336	
number	XXXX	Concentration limits: >= 25 %: Eye Irrit. 2, H319; >= 25 %: STOT SE 3, H335;	

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Nitrogen oxides (NO_x)
Hydrogen bromide gas
Zinc/zinc oxides
Combustible.

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

No data available

SECTION 6: Accidental release measures**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Do not flush with water.

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**

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Use explosion-proof equipment. **Advice on protection against fire and explosion**
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.
Never allow product to get in contact with water during storage.

Storage stability

Recommended storage temperature
2 - 8 °C

Store under inert gas. Dry residue is explosive. Test for peroxide formation periodically and before distillation. Dry residue is explosive. Store under inert gas. Test for peroxide formation periodically and before distillation.

Storage class (TRGS 510): 4.3: Hazardous materials, which set free flammable gases upon contact with water

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Tetrahydrofuran	109-99-9	TWA	50 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		
		STEL	100 ppm	USA. ACGIH Threshold Limit Values (TLV)
		Confirmed animal carcinogen with unknown relevance to humans Danger of cutaneous absorption		

		ST	250 ppm 735 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	200 ppm 590 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	200 ppm 590 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	200 ppm 590 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		STEL	250 ppm 735 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	200 ppm 590 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	250 ppm 735 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

Biological occupational exposure limits

Component	CAS-No.	Parameters	Value	Biological specimen	Basis
Tetrahydrofuran	109-99-9	Tetrahydrofuran	2 mg/l	Urine	ACGIH - Biological Exposure Indices (BEI)
	Remarks	End of shift (As soon as possible after exposure ceases)			

8.2 Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

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

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.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387)

respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	65.0 - 67.0 °C 149.0 - 152.6 °F
g) Flash point	-17 °C (1 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 11.8 %(V) Lower explosion limit: 1.8 %(V)
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	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 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapors may form explosive mixture with air.
Reacts violently with water.

10.4 Conditions to avoid

Heat, flames and sparks. Exposure to moisture.

10.5 Incompatible materials

Oxidizing agents, Oxygen

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Acute toxicity estimate Oral - 1,651 mg/kg
(Calculation method)

Inhalation: No data available

Acute toxicity estimate Dermal - 2,500 mg/kg
(Calculation method)
No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is

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identified as probable, possible or confirmed human carcinogen by IARC.

- NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard

No data available

11.2 Additional Information

Not available

Central nervous system depression, Cough, chest pain, Difficulty in breathing, Exposure to high airborne concentrations can cause anesthetic effects., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Components

Tetrahydrofuran

Acute toxicity

LD50 Oral - Rat - male and female - 1,650 mg/kg

Remarks:

(ECHA)

Symptoms: Irritation of mucous membranes

LC50 Inhalation - Rat - male and female - 4 h - > 16.9 mg/l

(US-EPA)

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

Inhalation: Irritating to respiratory system.

LD50 Dermal - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 72 h

(Draize Test)

Repeated or prolonged exposure may cause skin irritation and dermatitis, due to degreasing properties of the product.

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Eye irritation

Remarks:

(ECHA)
(Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

Germ cell mutagenicity

In vivo tests did not show mutagenic effects

In vitro mammalian cell gene mutation test

Chinese hamster ovary cells

Result: negative

Ames test

Salmonella typhimurium

Result: negative

Carcinogenicity

Suspected of causing cancer.

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No toxicity to reproduction

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation. - Respiratory system

May cause drowsiness or dizziness. - Nervous system

Acute oral toxicity - Irritation of mucous membranes

Acute inhalation toxicity - mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

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

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 Other adverse effects

No data available

Components

Tetrahydrofuran

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 2,160 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 3,485 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to bacteria	static test EC20 - activated sludge - ca. 800 mg/l - 0.5 h (OECD Test Guideline 209)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 3399 Class: 4.3 (3) Packing group: II
Proper shipping name: Organometallic substance, liquid, water-reactive, flammable (Tetrahydrofuran, 4-Cyanophenylzinc bromide)
Reportable Quantity (RQ): 1000 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 3399 Class: 4.3 (3) Packing group: II EMS-No: F-G, S-N
Proper shipping name: ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (Tetrahydrofuran, 4-Cyanophenylzinc bromide)

IATA

UN number: 3399 Class: 4.3 (3) Packing group: II
Proper shipping name: Organometallic substance, liquid, water-reactive, flammable (Tetrahydrofuran, 4-Cyanophenylzinc bromide)

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

	CAS-No.	Revision Date
Tetrahydrofuran	109-99-9	

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Tetrahydrofuran	109-99-9	
4-Cyanophenylzinc bromide	131379-14-1	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Tetrahydrofuran	109-99-9	
4-Cyanophenylzinc bromide	131379-14-1	

SECTION 16: Other information

Further information

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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