

## SAFETY DATA SHEET

Version 8.7  
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-Cyanobenzylzinc bromide solution

Product Number : 517380  
Brand : Aldrich  
CAS-No. : 135579-87-2

**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

May form explosive peroxides.

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## SECTION 3: Composition/information on ingredients

### 3.2 Mixtures

Formula :  $C_8H_6BrNZn$   
Molecular weight : 261.43 g/mol

| Component              |                   | Classification                                                                        | Concentration    |
|------------------------|-------------------|---------------------------------------------------------------------------------------|------------------|
| <b>Tetrahydrofuran</b> |                   |                                                                                       |                  |
| 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:<br>>= 25 %: Eye Irrit. 2,<br>H319; >= 25 %: STOT SE<br>3, H335; |                  |

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

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Carbon dioxide (CO<sub>2</sub>) Dry powder

## **Unsuitable extinguishing media**

Water Foam

### **5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Hydrogen bromide gas

Zinc/zinc 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.

### **5.4 Further information**

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.

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## **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.

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## **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

Tightly closed. Keep away from heat and sources of ignition.  
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. 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

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## 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<br>Danger of cutaneous absorption |                    |                                         |
|                 |          | STEL                                                                                           | 100 ppm            | USA. ACGIH Threshold Limit Values (TLV) |
|                 |          | Confirmed animal carcinogen with unknown relevance to humans<br>Danger of cutaneous absorption |                    |                                         |

|  |  |      |                                  |                                                                                         |
|--|--|------|----------------------------------|-----------------------------------------------------------------------------------------|
|  |  | ST   | 250 ppm<br>735 mg/m <sup>3</sup> | USA. NIOSH Recommended Exposure Limits                                                  |
|  |  | TWA  | 200 ppm<br>590 mg/m <sup>3</sup> | USA. NIOSH Recommended Exposure Limits                                                  |
|  |  | TWA  | 200 ppm<br>590 mg/m <sup>3</sup> | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants        |
|  |  | TWA  | 200 ppm<br>590 mg/m <sup>3</sup> | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000                           |
|  |  | STEL | 250 ppm<br>735 mg/m <sup>3</sup> | USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000                           |
|  |  | PEL  | 200 ppm<br>590 mg/m <sup>3</sup> | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
|  |  | STEL | 250 ppm<br>735 mg/m <sup>3</sup> | 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

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). Safety glasses

#### Skin protection

required

#### 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.

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## 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)<br>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

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Formation of peroxides possible.  
Vapors may form explosive mixture with air.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

No data available

### 10.4 Conditions to avoid

Warming.

Moisture.

### 10.5 Incompatible materials

Oxidizing agents, Oxygen

### 10.6 Hazardous decomposition products

Peroxides

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Mixture

##### Acute toxicity

Acute toxicity estimate Oral - 1,651 mg/kg

(Calculation method)

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

Acute toxicity estimate Dermal - 2,500 mg/kg

(Calculation method)

No data available

##### Skin corrosion/irritation

No data available

##### Serious eye damage/eye irritation

Mixture causes serious eye irritation.

##### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

##### Carcinogenicity

Evidence of a carcinogenic effect.

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**

### **Specific target organ toxicity - single exposure**

Mixture may cause respiratory irritation.

Mixture may cause drowsiness or dizziness.

### **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.

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

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

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## **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

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#### 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<br>(OECD Test Guideline 203) |
| Toxicity to daphnia and other aquatic invertebrates | static test EC50 - Daphnia magna (Water flea) - 3,485 mg/l - 48 h<br>(OECD Test Guideline 202)                 |
| Toxicity to bacteria                                | static test EC20 - activated sludge - ca. 800 mg/l - 0.5 h<br>(OECD Test Guideline 209)                        |

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### SECTION 13: Disposal considerations

#### 13.1 Waste treatment methods

##### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

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### 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-Cyanobenzylzinc 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-Cyanobenzylzinc bromide)

#### IATA

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

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## 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-Cyanobenzylzinc bromide | 135579-87-2 |               |

### New Jersey Right To Know Components

|                           | CAS-No.     | Revision Date |
|---------------------------|-------------|---------------|
| Tetrahydrofuran           | 109-99-9    |               |
| 4-Cyanobenzylzinc bromide | 135579-87-2 |               |

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## SECTION 16: Other information

### Further information

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](http://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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