

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

1.1 Product identifier  
Trade name

**4-Cyanobutylzinc bromide, 0.5M in THF, packaged under Argonin resealable ChemSeal bottles**

Stock number:

H58897

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

Identified use:

SU24 Scientific research and development

1.3 Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar GmbH & Co.KG  
A Johnson Matthey Company  
Zeppelinstr. 7b  
76185 Karlsruhe / Germany  
Tel: +49 (0) 721 84007 280  
Fax: +49 (0) 721 84007 300  
Email: tech@alfa.com  
www.alfa.com

Informing department:

Product safety Tel + +049 (0) 7275 988687-0

1.4 Emergency telephone number:

Carechem 24: +44 (0) 1235 239 670 (Multi-language emergency number)  
Poison Information Center Mainz  
www.giftinfo.uni-mainz.de Telephone: +49(0)6131/19240

**SECTION 2: Hazards identification**

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008



GHS02 flame

Flam. Liq. 2 H225 Highly flammable liquid and vapour.

Water-react. 2 H261 In contact with water releases flammable gases.



GHS08 health hazard

Carc. 2 H351 Suspected of causing cancer.



GHS05 corrosion

Skin Corr. 1B H314 Causes severe skin burns and eye damage.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

STOT SE 3 H335 May cause respiratory irritation.

Classification according to Directive 67/548/EEC or Directive 1999/45/EC

C; Corrosive

R34 Causes burns.

Xn; Harmful

R22 Harmful if swallowed.

Xi; Irritant

R37 Irritating to respiratory system.

F; Highly flammable

R11-15 Highly flammable. Contact with water liberates extremely flammable gases.

R19 May form explosive peroxides.

**Information concerning particular hazards for human and environment:**

The product has to be labelled due to the calculation procedure of the "General Classification guideline for preparations of the EU" in the latest valid version.

**Other hazards that do not result in classification**

No information known.

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008

Hazard pictograms

Signal word

Hazard-determining components of labelling:

Hazard statements

Precautionary statements

Additional information:

2.3 Other hazards

Results of PBT and vPvB assessment

PBT:

Not applicable.

vPvB:

Not applicable.

The product is classified and labelled according to the CLP regulation.

GHS02, GHS05, GHS07, GHS08  
Danger

Tetrahydrofuran

4-Cyanobutylzinc bromide

H225 Highly flammable liquid and vapour.

H261 In contact with water releases flammable gases.

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H351 Suspected of causing cancer.

H335 May cause respiratory irritation.

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

P231+P232 Handle under inert gas. Protect from moisture.

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

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

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

EUH019 May form explosive peroxides.

**Trade name 4-Cyanobutylzinc bromide, 0.5M in THF, packaged under Argonin resealable ChemSeal bottles**

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### SECTION 3: Composition/information on ingredients

#### 3.2 Mixtures

##### Dangerous components:

CAS: 109-99-9 EINECS: 203-726-8	Tetrahydrofuran	☒ Xn R40; ☒ Xi R36/37; ☒ F R11 R19	88,6%
CAS: 226570-68-9	4-Cyanobutylzinc bromide	☒ Flam. Liq. 2, H225; ☒ Carc. 2, H351; ☒ Eye Irrit. 2, H319; STOT SE 3, H335 ☒ T R25; ☒ C R34; ☒ F R15 ☒ Water-react. 1, H260; ☒ Acute Tox. 3, H301; ☒ Skin Corr. 1B, H314	11,4%

##### Additional information

None known.

### SECTION 4: First aid measures

#### 4.1 Description of first aid measures

##### General information

Instantly remove any clothing soiled by the product.  
Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

##### After inhalation

Seek immediate medical advice.

##### After skin contact

Instantly wash with water and soap and rinse thoroughly.

##### After eye contact

Seek immediate medical advice.

##### After swallowing

Rinse opened eye for several minutes under running water. Then consult doctor.

#### 4.2 Most important symptoms and effects, both acute and delayed

Seek medical treatment.

#### 4.3 Indication of any immediate medical attention and special treatment needed

No further relevant information available.

No further relevant information available.

### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media

##### Suitable extinguishing agents

In case of fire, use sand, carbon dioxide or powdered extinguishing agent. Never use water.

##### For safety reasons unsuitable extinguishing agents

Water.

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

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Hydrogen cyanide (HCN)

Nitrogen oxides (NOx)

Hydrogen bromide (HBr)

Metal oxide

#### 5.3 Advice for firefighters

##### Protective equipment:

Wear self-contained breathing apparatus.

Wear full protective suit.

### SECTION 6: Accidental release measures

#### 6.1 Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

Ensure adequate ventilation

Keep away from ignition sources

#### 6.2 Environmental precautions:

Do not allow material to be released to the environment without proper governmental permits.

Do not allow product to reach sewage system or water bodies.

Do not allow to enter the ground/soil.

#### 6.3 Methods and material for containment and cleaning up:

Keep away from ignition sources.

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Use neutralizing agent.

Dispose of contaminated material as waste according to item 13.

Ensure adequate ventilation.

Do not flush with water or aqueous cleansing agents

Keep away from ignition sources.

#### Prevention of secondary hazards:

#### 6.4 Reference to other sections

See Section 7 for information on safe handling

See section 8 for information on personal protection equipment.

See Section 13 for information on disposal.

### SECTION 7: Handling and storage

#### 7.1 Precautions for safe handling

Handle under dry protective gas.

Keep containers tightly sealed.

Ensure good ventilation/exhaustion at the workplace.

Open and handle container with care.

#### Information about protection against explosions and fires:

Protect against electrostatic charges.

Fumes can combine with air to form an explosive mixture.

Do not distill to dryness.

Explosive peroxides may form, handle container cautiously.

#### 7.2 Conditions for safe storage, including any incompatibilities

##### Storage

##### Requirements to be met by storerooms and containers:

Refrigerate

##### Information about storage in one common storage facility:

Store away from air.

Protect from heat.

Store away from strong bases.

Store away from oxidizing agents.

#### Further information about storage conditions:

Store under dry inert gas.

This product is air sensitive.

Avoid contact with air / oxygen (formation of peroxide).

Store in a locked cabinet or with access restricted to technical experts or their assistants.

Refrigerate

#### 7.3 Specific end use(s)

Check container pressure periodically to prevent explosive peroxides.

No further relevant information available.

**Trade name 4-Cyanobutylzinc bromide, 0.5M in THF, packaged under Argonin resealable ChemSeal bottles**

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### SECTION 8: Exposure controls/personal protection

**Additional information about design of technical systems:** Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

#### 8.1 Control parameters

**Components with critical values that require monitoring at the workplace:**

##### 109-99-9 Tetrahydrofuran (88,6%)

AGW (Germany)	150 mg/m <sup>3</sup> , 50 ppm 2(l);DFG, EU, H, Y
PEL (USA)	590 mg/m <sup>3</sup> , 200 ppm
REL (USA)	Short-term value: 735 mg/m <sup>3</sup> , 250 ppm Long-term value: 590 mg/m <sup>3</sup> , 200 ppm
TLV (USA)	Short-term value: 295 mg/m <sup>3</sup> , 100 ppm Long-term value: 147 mg/m <sup>3</sup> , 50 ppm Skin

**Ingredients with biological limit values:**

##### 109-99-9 Tetrahydrofuran (88,6%)

BGW (Germany)	2 mg/l U b Tetrahydrofuran
BEI (USA)	2 mg/L urine end of shift Tetrahydrofuran

**Additional information:** No data

#### 8.2 Exposure controls

##### Personal protective equipment

##### General protective and hygienic measures

The usual precautionary measures should be adhered to in handling the chemicals.  
Keep away from foodstuffs, beverages and food.  
Instantly remove any soiled and impregnated garments.  
Wash hands during breaks and at the end of the work.  
Do not inhale dust / smoke / mist.  
Avoid contact with the eyes and skin.  
Maintain an ergonomically appropriate working environment.  
Use breathing protection with high concentrations.  
Check protective gloves prior to each use for their proper condition.  
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

##### Breathing equipment:

##### Protection of hands:

##### Material of gloves

##### Penetration time of glove material

##### Eye protection:

##### Body protection:

Impervious gloves  
Not determined  
Tightly sealed safety glasses.  
Full face protection  
Protective work clothing.

### SECTION 9: Physical and chemical properties

#### 9.1 Information on basic physical and chemical properties

##### General Information

##### Appearance:

Form:	Liquid
Colour:	Yellow to brown to black
Smell:	Not determined
Odour threshold:	Not determined.

**pH-value:** Not determined.

##### Change in condition

Melting point/Melting range:	Not determined
Boiling point/Boiling range:	Not determined
Sublimation temperature / start:	Not determined
Inflammability (solid, gaseous)	Not determined.
Ignition temperature:	230 °C
Decomposition temperature:	Not determined
Self-inflammability:	Product is not selfigniting.

##### Danger of explosion:

May form explosive peroxides.  
Do not distill to dryness.

##### Critical values for explosion:

Lower:	1,5 Vol %
Upper:	12,0 Vol %
Steam pressure at 20 °C:	200 hPa
Density at 20 °C	0,971 g/cm <sup>3</sup>
Relative density	Not determined.
Vapour density	Not determined.
Evaporation rate	Not determined.
Solubility in / Miscibility with	
Water:	Contact with water releases flammable gases
Partition coefficient (n-octanol/water):	Not determined.
Viscosity:	
dynamic:	Not determined.
kinematic:	Not determined.

##### Solvent content:

**Organic solvents:** 88,6 %

**Solids content:** 11,4 %

**9.2 Other information** No further relevant information available.

### SECTION 10: Stability and reactivity

#### 10.1 Reactivity

In contact with water releases flammable gases which may ignite spontaneously.  
May form explosive peroxides.

#### 10.2 Chemical stability

Stable under recommended storage conditions.

#### Thermal decomposition / conditions to be avoided:

No decomposition if used and stored according to specifications.

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**Trade name 4-Cyanobutylzinc bromide, 0.5M in THF, packaged under Argonin resealable ChemSeal bottles**

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<b>10.3 Possibility of hazardous reactions</b>	Reacts with strong oxidizing agents Contact with water releases flammable gases
<b>10.5 Incompatible materials:</b>	Forms peroxides Air Bases Oxidizing agents Heat Water/moisture
<b>10.6 Hazardous decomposition products:</b>	Carbon monoxide and carbon dioxide Hydrogen cyanide (prussic acid) Nitrogen oxides (NOx) Hydrogen bromide Metal oxide

**SECTION 11: Toxicological information**

**11.1 Information on toxicological effects**

<b>Acute toxicity:</b>	Harmful if swallowed. Swallowing will lead to a strong caustic effect on mouth and throat and to the danger of perforation of esophagus and stomach. The Registry of Toxic Effects of Chemical Substances (RTECS) contains acute toxicity data for components in this product.
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**LD/LC50 values that are relevant for classification:**

**109-99-9 Tetrahydrofuran**

Oral	LD50	1650 mg/kg (rat)
Inhalative	LC50/2H	72000 mg/m <sup>3</sup> /2H (rat)

<b>Skin irritation or corrosion:</b>	Causes severe skin burns.
<b>Eye irritation or corrosion:</b>	Causes serious eye damage.
<b>Sensitization:</b>	No sensitizing effect known.
<b>Germ cell mutagenicity:</b>	The Registry of Toxic Effects of Chemical Substances (RTECS) contains mutation data for components in this product.
<b>Carcinogenicity:</b>	ACGIH A3: Animal carcinogen: Agent is carcinogenic in experimental animals at a relatively high dose, by route(s) of administration, at site(s), of histologic type(s), or by mechanism(s) not considered relevant to worker exposure. Available epidemiologic studies do not confirm an increased risk of cancer in exposed humans. Available evidence suggests that the agent is not likely to cause cancer in humans except under uncommon or unlikely routes or levels of exposure. The Registry of Toxic Effects of Chemical Substances (RTECS) contains tumorigenic and/or carcinogenic and/or neoplastic data for this product.
<b>Reproductive toxicity:</b>	The Registry of Toxic Effects of Chemical Substances (RTECS) contains reproductive data for components in this product.
<b>Specific target organ system toxicity - repeated exposure:</b>	No effects known.
<b>Specific target organ system toxicity - single exposure:</b>	May cause respiratory irritation.
<b>Aspiration hazard:</b>	No effects known.
<b>Experience with humans:</b>	The Registry of Toxic Effects of Chemical Substances (RTECS) contains multiple dose toxicity data for components in this product.
<b>Additional toxicological information:</b>	To the best of our knowledge the acute and chronic toxicity of this substance is not fully known. Harmful if swallowed. The product shows the following dangers according to the calculation method of the General EC Classification Guidelines for Preparations as issued in the latest version: Harmful Corrosive Irritant

**SECTION 12: Ecological information**

<b>12.1 Toxicity</b>	No further relevant information available.
<b>Aquatic toxicity:</b>	No further relevant information available.
<b>12.2 Persistence and degradability</b>	No further relevant information available.
<b>12.3 Bioaccumulative potential</b>	No further relevant information available.
<b>12.4 Mobility in soil</b>	No further relevant information available.
<b>Additional ecological information:</b>	
<b>General notes:</b>	Do not allow material to be released to the environment without proper governmental permits. Water hazard class 1 (Self-assessment): slightly hazardous for water. Do not allow undiluted product or large quantities of it to reach ground water, water bodies or sewage system. Avoid transfer into the environment.
<b>12.5 Results of PBT and vPvB assessment</b>	
<b>PBT:</b>	Not applicable.
<b>vPvB:</b>	Not applicable.
<b>12.6 Other adverse effects</b>	No further relevant information available.

**SECTION 13: Disposal considerations**

<b>13.1 Waste treatment methods</b>	
<b>Recommendation</b>	Hand over to disposers of hazardous waste. Must be specially treated under adherence to official regulations. Consult state, local or national regulations for proper disposal.
<b>Uncleaned packagings:</b>	
<b>Recommendation:</b>	Disposal must be made according to official regulations.

**SECTION 14: Transport information**

<b>UN-Number</b>	
<b>ADR, IMDG, IATA</b>	UN3399
<b>14.2 UN proper shipping name</b>	
<b>ADR</b>	3399 ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE
<b>IMDG, IATA</b>	ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE

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DE/E

**Safety data sheet**  
according to 1907/2006/EC, Article 31

Printing date 02.07.2013

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Trade name **4-Cyanobutylzinc bromide, 0.5M in THF, packaged under Argonin resealable ChemSeal bottles**

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**14.3 Transport hazard class(es)**

ADR

Class  
Label  
IMDG, IATA4.3 (WF1) Substances which, in contact with water, emit flammable gases.  
4.3+3Class  
Label4.3 Substances which, in contact with water, emit flammable gases.  
4.3+3Packing group  
ADR, IMDG, IATA

II

14.5 Environmental hazards:  
Marine pollutant:

No

14.6 Special precautions for user  
Kemler Number:Warning: Substances which, in contact with water, emit flammable gases.  
32314.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC  
Code

Not applicable.

Transport/Additional information:

ADR

Excepted quantities (EQ):  
Limited quantities (LQ)  
Transport category  
Tunnel restriction codeE2  
500 ml  
0  
D/E

UN "Model Regulation":

UN3399, ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE,  
FLAMMABLE, 4.3 (3), II**SECTION 15: Regulatory information**

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

Australian Inventory of Chemical Substances

109-99-9 | Tetrahydrofuran

Standard for the Uniform Scheduling of Drugs and Poisons

None of the ingredients is listed.

National regulations

Information about limitation of use:

For use only by technically qualified individuals.  
Employment restrictions concerning young persons must be observed.  
Not applicable

Classification according to VbF:

Technical instructions (air):

Class	Share in %
NK	88,6

Water hazard class:

Water hazard class 1 (Self-assessment): slightly hazardous for water.

Other regulations, limitations and prohibitive regulations

ELINCS (European List of Notified Chemical Substances)

None of the ingredients is listed.

Substances of very high concern (SVHC) according to REACH, Article 57

None of the ingredients are listed.

REACH - Pre-registered substances

109-99-9 | Tetrahydrofuran

15.2 Chemical safety assessment:

A Chemical Safety Assessment has not been carried out.

**SECTION 16: Other information**

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Relevant phrases

H225 Highly flammable liquid and vapour.  
 H260 In contact with water releases flammable gases which may ignite spontaneously.  
 H301 Toxic if swallowed.  
 H314 Causes severe skin burns and eye damage.  
 H319 Causes serious eye irritation.  
 H335 May cause respiratory irritation.  
 H351 Suspected of causing cancer.

R11 Highly flammable.  
 R15 Contact with water liberates extremely flammable gases.  
 R19 May form explosive peroxides.  
 R25 Toxic if swallowed.  
 R34 Causes burns.  
 R36/37 Irritating to eyes and respiratory system.  
 R40 Limited evidence of a carcinogenic effect.

Department issuing data specification sheet:

Abbreviations and acronyms:

Health, Safety and Environmental Department.  
 ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)  
 IMDG: International Maritime Code for Dangerous Goods  
 IATA: International Air Transport Association  
 GHS: Globally Harmonized System of Classification and Labelling of Chemicals  
 VbF: Verordnung über brennbare Flüssigkeiten, Österreich (Ordinance on the storage of combustible liquids, Austria)  
 LC50: Lethal concentration, 50 percent  
 LD50: Lethal dose, 50 percent

DE/E