

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

Revision: 09.05.2013

Printing date 02.07.2013

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifier**

Trade name

**4-Fluorophenylzinc bromide, 0.5M in THF**

Stock number:

H58780

**1.2 Relevant identified uses of the substance**

or mixture and uses advised against.

No further relevant information available.

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

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

R40: Limited evidence of a carcinogenic effect.



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

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

Signal word

GHS02, GHS05, GHS07, GHS08  
Danger

Hazard-determining components of labelling:

Tetrahydrofuran

4-Fluorophenylzinc bromide

H225 Highly flammable liquid and vapour.

H261 In contact with water releases flammable gases.

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.

**Additional information:****2.3 Other hazards**

Results of PBT and vPvB assessment

PBT:

Not applicable.

vPvB:

Not applicable.

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Trade name **4-Fluorophenylzinc bromide, 0.5M in THF**

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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 ☒ Flam. Liq. 2, H225; ☒ Carc. 2, H351; ☒ Eye Irrit. 2, H319; STOT SE 3, H335	88,0%
CAS: 181705-93-1	4-Fluorophenylzinc bromide ☒ C R34; ☒ F R15 ☒ Water-react. 1, H260; ☒ Skin Corr. 1B, H314	12,0%

**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.  
Instantly wash with water and soap and rinse thoroughly.

**After skin contact**

Seek immediate medical advice.  
Rinse opened eye for several minutes under running water. Then consult doctor.

**After eye contact**

Seek medical treatment.

**After swallowing****4.2 Most important symptoms and effects, both acute and delayed**

No further relevant information available.

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

No further relevant information available.

**SECTION 5: Firefighting measures****5.1 Extinguishing media**

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

**Suitable extinguishing agents**

Water.

**For safety reasons unsuitable extinguishing agents****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 fluoride (HF)  
Hydrogen bromide (HBr)  
Metal oxide

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus.  
Wear full protective suit.

**Protective equipment:****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:**

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.

**Prevention of secondary hazards:**

Do not flush with water or aqueous cleansing agents  
Keep away from ignition sources.

**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.

DE/E

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Trade name **4-Fluorophenylzinc bromide, 0.5M in THF**

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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 (88,0%)**

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 (88,0%)**

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.

**Breathing equipment:****Protection of hands:**

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.

**Material of gloves**

Impervious gloves

**Penetration time of glove material**

Not determined

**Eye protection:**

Tightly sealed safety glasses.

**Body protection:**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	0,992 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: 88,0 %

**Solids content:**

12,0 %

**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-Fluorophenylzinc bromide, 0.5M in THF**

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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 fluoride Hydrogen bromide Metal oxide

**SECTION 11: Toxicological information**
**11.1 Information on toxicological effects**

**Acute toxicity:** 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.

**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>	Suspected of causing cancer. EPA-S: Suggestive evidence of carcinogenicity, but not sufficient to assess human carcinogenic potential. 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. 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: 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>	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>General notes:</b>	
<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>	Hand over to disposers of hazardous waste.
<b>Recommendation</b>	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> ADR, IMDG, IATA	UN3399
<b>14.2 UN proper shipping name</b> ADR	3399 ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (4-Fluorophenylzinc bromide, TETRAHYDROFURAN)
<b>IMDG, IATA</b>	ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE (4-Fluorophenylzinc bromide, TETRAHYDROFURAN)
<b>14.3 Transport hazard class(es)</b> ADR	
 	
<b>Class</b>	4.3 (WF1) Substances which, in contact with water, emit flammable gases.

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Label  
IMDG, IATA

4.3+3

Class  
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

Warning: Substances which, in contact with water, emit flammable gases.

Kemler Number:

323

EMS Number:

F-G,S-M

14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC  
Code

Not applicable.

Transport/Additional information:

ADR

Excepted quantities (EQ):

E2

Limited quantities (LQ)

500 ml

Transport category

0

Tunnel restriction code

D/E

UN "Model Regulation":

UN3399, ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE,  
FLAMMABLE (4-Fluorophenylzinc bromide, TETRAHYDROFURAN), 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	88,0

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.  
 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.  
 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