

**SAFETY DATA SHEET**  
4-FLUOROPHENYLZINC BROMIDE IN THF 0.5MOL

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**Compilation date:** 28/05/2015  
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**Section 1: Identification of the substance/mixture and of the company/undertaking**

**1.1. Product identifier**

**Product name:** 4-FLUOROPHENYLZINC BROMIDE IN THF 0.5MOL  
**CAS number:** 181705-93-1  
**Product code:** PC1152

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

**1.3. Details of the supplier of the safety data sheet**

**Company name:** Apollo Scientific Ltd  
Units 3 & 4  
Parkway  
Denton  
Manchester  
M34 3SG  
UK  
**Tel:** 0161 337 9971  
**Fax:** 0161 336 6932  
**Email:** david.tideswell@apolloscientific.co.uk

**1.4. Emergency telephone number**

**Section 2: Hazards identification**

**2.1. Classification of the substance or mixture**

**Classification under CLP:** Flam. Liq. 2: H225; Water-react. 2: H261; Carc. 2: H351; Skin Corr. 1B: H314; STOT SE 3: H335; -: EUH019

**Classification under CHIP:** F: R11; -: R15; -: R19; C: R34; Xi: R37; Xn: R40

**Most important adverse effects:** Highly flammable liquid and vapour. In contact with water releases flammable gases.  
Causes severe skin burns and eye damage. May cause respiratory irritation. Suspected of causing cancer. May form explosive peroxides.

**2.2. Label elements**

**Label elements:**

**Hazard statements:** H225: Highly flammable liquid and vapour.  
H261: In contact with water releases flammable gases.  
H314: Causes severe skin burns and eye damage.  
H335: May cause respiratory irritation.

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H351: Suspected of causing cancer.

EUH019: May form explosive peroxides.

**Signal words:** Danger

**Hazard pictograms:** GHS02: Flame

GHS05: Corrosion

GHS07: Exclamation mark

GHS08: Health hazard



**Precautionary statements:** P210: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

P260: Do not breathe dust.

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

P308+313: IF exposed or concerned: Get medical advice/attention.

P310: Immediately call a POISON CENTER/doctor/.

### 2.3. Other hazards

**Other hazards:** In use, may form flammable / explosive dust-air mixture.

**PBT:** This product is not identified as a PBT/vPvB substance.

## Section 3: Composition/information on ingredients

### 3.1. Substances

**Chemical identity:** 4-FLUOROPHENYLZINC BROMIDE IN THF 0.5MOL

**CAS number:** 181705-93-1

## Section 4: First aid measures

### 4.1. Description of first aid measures

**Skin contact:** Remove all contaminated clothes and footwear immediately unless stuck to skin. Drench the affected skin with running water for 10 minutes or longer if substance is still on skin. Transfer to hospital if there are burns or symptoms of poisoning.

**Eye contact:** Bathe the eye with running water for 15 minutes. Transfer to hospital for specialist examination. Consult a doctor.

**Ingestion:** Do not induce vomiting. If conscious, give half a litre of water to drink immediately. Consult a doctor.

**Inhalation:** Remove casualty from exposure ensuring one's own safety whilst doing so. Consult a doctor.

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

**Skin contact:** There may be mild irritation at the site of contact.

**Eye contact:** There may be irritation and redness.

[cont...]

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**Ingestion:** There may be irritation of the throat.

**Inhalation:** There may be irritation of the throat with a feeling of tightness in the chest.

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

**Section 5: Fire-fighting measures**

**5.1. Extinguishing media**

**Extinguishing media:** Carbon dioxide, dry chemical powder, foam. Suitable extinguishing media for the surrounding fire should be used.

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

**Exposure hazards:** Corrosive. Highly flammable. May form flammable / explosive dust-air mixture. In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Hydrogen bromide (HBr). Hydrogen fluoride (HF). Zinc oxides.

**5.3. Advice for fire-fighters**

**Advice for fire-fighters:** Wear self-contained breathing apparatus. Wear protective clothing to prevent contact with skin and eyes.

**Section 6: Accidental release measures**

**6.1. Personal precautions, protective equipment and emergency procedures**

**Personal precautions:** Refer to section 8 of SDS for personal protection details. Notify the police and fire brigade immediately. Eliminate all sources of ignition.

**6.2. Environmental precautions**

**Environmental precautions:** Do not discharge into drains or rivers.

**6.3. Methods and material for containment and cleaning up**

**Clean-up procedures:** Transfer to a closable, labelled salvage container for disposal by an appropriate method. Do not use equipment in clean-up procedure which may produce sparks.

**6.4. Reference to other sections**

**Section 7: Handling and storage**

**7.1. Precautions for safe handling**

**Handling requirements:** Smoking is forbidden. Keep container tightly closed. Close container after use or when empty. Use non-sparking tools. Ensure there is sufficient ventilation of the area. Avoid the formation or spread of dust in the air. Only use in fume hood.

**7.2. Conditions for safe storage, including any incompatibilities**

**Storage conditions:** Store in a cool, well ventilated area. Keep container tightly closed. Keep away from sources of ignition. Prevent the build up of electrostatic charge in the immediate area. Ensure lighting and electrical equipment are not a source of ignition. Air sensitive. Light

[cont...]

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Sensitive. Store under Argon. Recommended storage temp 2-8 °C. Dry residue is explosive. Test for peroxide formation periodically and before distillation.

**Suitable packaging:** Must only be kept in original packaging.

### 7.3. Specific end use(s)

**Specific end use(s):** No data available.

## Section 8: Exposure controls/personal protection

### 8.1. Control parameters

**Workplace exposure limits:** No data available.

### DNEL/PNEC Values

**DNEL / PNEC** No data available.

### 8.2. Exposure controls

**Engineering measures:** Ensure there is sufficient ventilation of the area. Ensure lighting and electrical equipment are not a source of ignition.

**Respiratory protection:** Respiratory protective device with particle filter.

**Hand protection:** Protective gloves.

**Eye protection:** Safety glasses. Ensure eye bath is to hand.

**Skin protection:** Protective clothing.

## Section 9: Physical and chemical properties

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

**State:** Liquid

**Colour:** Yellow to Brown to Black

**Boiling point/range °C:** 65-67

**upper:** 11.8

**Autoflammability °C:** 321

**Flammability limits %: lower:** 1.8

**Flash point °C:** -17

**Relative density:** 0.992 g/ml

### 9.2. Other information

**Other information:** No data available.

## Section 10: Stability and reactivity

### 10.1. Reactivity

**Reactivity:** Stable under recommended transport or storage conditions.

### 10.2. Chemical stability

**Chemical stability:** Stable under normal conditions. Stable at room temperature.

### 10.3. Possibility of hazardous reactions

**Hazardous reactions:** Hazardous reactions will not occur under normal transport or storage conditions.

[cont...]

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### 10.4. Conditions to avoid

**Conditions to avoid:** Heat. Hot surfaces. Sources of ignition. Flames.

### 10.5. Incompatible materials

**Materials to avoid:** Strong oxidising agents. Strong acids.

### 10.6. Hazardous decomposition products

**Haz. decomp. products:** In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Hydrogen bromide gas (HBr). Hydrogen fluoride (HF). Zinc oxides.

## Section 11: Toxicological information

### 11.1. Information on toxicological effects

#### Toxicity values:

Route	Species	Test	Value	Units
ORAL	RAT	LD50	1650	mg/kg
INHALATION	RAT	2H LC50	72000	mg/m3

#### Relevant hazards for substance:

Hazard	Route	Basis
Skin corrosion/irritation	DRM	Based on test data
Serious eye damage/irritation	OPT	Based on test data
Carcinogenicity	--	Based on test data
STOT-single exposure	INH	Based on test data

### Symptoms / routes of exposure

**Skin contact:** There may be mild irritation at the site of contact.

**Eye contact:** There may be irritation and redness.

**Ingestion:** There may be irritation of the throat.

**Inhalation:** There may be irritation of the throat with a feeling of tightness in the chest.

## Section 12: Ecological information

### 12.1. Toxicity

**Ecotoxicity values:** No data available.

### 12.2. Persistence and degradability

**Persistence and degradability:** No data available.

### 12.3. Bioaccumulative potential

**Bioaccumulative potential:** No data available.

[cont...]

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### 12.4. Mobility in soil

**Mobility:** No data available.

### 12.5. Results of PBT and vPvB assessment

**PBT identification:** This product is not identified as a PBT/vPvB substance.

### 12.6. Other adverse effects

**Other adverse effects:** No data available.

## Section 13: Disposal considerations

### 13.1. Waste treatment methods

**Disposal operations:** Transfer to a suitable container and arrange for collection by specialised disposal company. MATERIAL SHOULD BE DISPOSED OF IN ACCORDANCE WITH LOCAL, STATE AND FEDERAL REGULATIONS

**Disposal of packaging:** Dispose of as special waste in compliance with local and national regulations Observe all federal, state and local environmental regulations.

**NB:** The user's attention is drawn to the possible existence of regional or national regulations regarding disposal.

## Section 14: Transport information

### 14.1. UN number

**UN number:** UN3399

### 14.2. UN proper shipping name

**Shipping name:** ORGANOMETALLIC SUBSTANCE, LIQUID, WATER-REACTIVE, FLAMMABLE

### 14.3. Transport hazard class(es)

**Transport class:** 4.3 (3)

### 14.4. Packing group

**Packing group:** II

### 14.5. Environmental hazards

**Environmentally hazardous:** No

**Marine pollutant:** No

### 14.6. Special precautions for user

**Tunnel code:** D/E

**Transport category:** 0

## Section 15: Regulatory information

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

[cont...]

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### 15.2. Chemical Safety Assessment

**Chemical safety assessment:** A chemical safety assessment has not been carried out for the substance or the mixture by the supplier.

## Section 16: Other information

### Other information

**Other information:** This safety data sheet is prepared in accordance with Commission Regulation (EU) No 453/2010.

\* Data predicted using computational software. Toxtree - Toxic Hazard Estimation by decision tree approach. [http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?](http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?c=TOXTREE)

c=TOXTREE

~ Data predicted using computational software ACD/ToxSuite v 2.95.1 Copyright 1994-2009 ACD/labs, Copyright 2001-2009 Pharma Algorithms, Inc, Advanced Chemistry Development, Inc (ACD/Labs). [http://www.acdlabs.com/products/pc\\_admet/tox/tox/](http://www.acdlabs.com/products/pc_admet/tox/tox/)

**Phrases used in s.2 and s.3:** EUH019: May form explosive peroxides.  
H225: Highly flammable liquid and vapour.  
H261: In contact with water releases flammable gases.  
H314: Causes severe skin burns and eye damage.  
H335: May cause respiratory irritation.  
H351: Suspected of causing cancer <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>.  
R11: Highly flammable.  
R15: Contact with water liberates extremely flammable gases.  
R19: May form explosive peroxides.  
R34: Causes burns.  
R37: Irritating to respiratory system.  
R40: Limited evidence of a carcinogenic effect.

**Legend to abbreviations:** PNEC = predicted no effect level  
DNEL = derived no effect level  
LD50 = median lethal dose  
LC50 = median lethal concentration  
EC50 = median effective concentration  
IC50 = median inhibitory concentration  
dw = dry weight  
bw = body weight  
cc = closed cup  
oc = open cup  
MUS = mouse  
GPG = guinea pig

[cont...]

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RBT = rabbit

HAM = hamster

HMN = human

MAM = mammal

PGN = pigeon

IVN = intravenous

SCU = subcutaneous

SKN = skin

DRM = dermal

OCC = ocular/corneal

PCP = physico-chemical properties

**Legal disclaimer:** The material is intended for research purposes only and should be handled exclusively by those who have been fully trained in safety, laboratory and chemical handling procedures. The above information is believed to be correct to the best of our knowledge. The above information is believed to be correct to the best of our knowledge at the date of its publication, but should not be considered to be all inclusive. It should be used only as a guide for safe handling, storage, transportation and disposal. We cannot guarantee that the hazards detailed in this document are the only hazards that exist for this product. This is not a warranty and Apollo Scientific Ltd shall not be held liable for any damage resulting from handling or from contact with the above product.