

## SAFETY DATA SHEET

1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI(TETRAFLUOROBORATE), 50% ON ALUMINA

Page: 1

Compilation date: 23/10/2007

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Revision No: 2

### Section 1: Identification of the substance/mixture and of the company/undertaking

#### 1.1. Product identifier

**Product name:** 1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI  
(TETRAFLUOROBORATE), 50% ON ALUMINA

**CAS number:** 162241-33-0

**Index number:** 603-215-00-3

**Product code:** PC6854

**Synonyms:** ACCUFLUOR NFTH™

#### 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 CHIP:** Xi: R41; Sens.: R43; N: R50/53; Xn: R48/22

**Classification under CLP:** Eye Dam. 1: H318; Aquatic Chronic 1: H410; STOT RE 2: H373; Skin Sens. 1: H317

**Most important adverse effects:** Risk of serious damage to eyes. May cause sensitisation by skin contact. Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.  
Harmful: danger of serious damage to health by prolonged exposure if swallowed.

#### 2.2. Label elements

**Label elements under CLP:**

**Hazard statements:** H373: May cause damage to organs through prolonged or repeated exposure.

H318: Causes serious eye damage.

H410: Very toxic to aquatic life with long lasting effects.

## SAFETY DATA SHEET

1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI(TETRAFLUOROBORATE), 50% ON ALUMINA

Page: 2

**Signal words:** Danger

**Hazard pictograms:** GHS08: Health hazard

GHS05: Corrosion

GHS07: Exclamation mark

GHS09: Environmental



**Precautionary statements:** P260: Do not breathe dust.

P271: Use only outdoors or in a well-ventilated area.

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

**Label elements under CHIP:**

**Hazard symbols:** Dangerous for the environment.

Harmful.



**Risk phrases:** R41: Risk of serious damage to eyes.

R43: May cause sensitisation by skin contact.

R50/53: Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

R48/22: Harmful: danger of serious damage to health by prolonged exposure if swallowed.

**Safety phrases:** S22: Do not breathe dust.

S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

S36/37/39: Wear suitable protective clothing, gloves and eye / face protection.

### 2.3. Other hazards

**PBT:** This substance is not identified as a PBT substance.

## Section 3: Composition/information on ingredients

### 3.1. Substances

**Chemical identity:** 1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI  
(TETRAFLUOROBORATE), 50% ON ALUMINA

## 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. Consult a doctor.

[cont...]

## SAFETY DATA SHEET

1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI(TETRAFLUOROBORATE), 50% ON ALUMINA

Page: 3

**Eye contact:** Bathe the eye with running water for 15 minutes. Consult a doctor.

**Ingestion:** Wash out mouth with water. 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 irritation and redness at the site of contact.

**Eye contact:** There may be irritation and redness. The eyes may water profusely. Eye-Rabbit-Severe eye irritation -24h

**Ingestion:** There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

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

**Delayed / immediate effects:** No data available.

### 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:** In combustion emits toxic fumes. Nitrogen oxides (NO<sub>x</sub>). Hydrogen fluoride (HF). Hydrogen cyanide (HCN). Borane/boron oxides. Aluminium 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. If outside do not approach from downwind. If outside keep bystanders upwind and away from danger point. Mark out the contaminated area with signs and prevent access to unauthorised personnel.

### 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.

[cont...]

# SAFETY DATA SHEET

1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI(TETRAFLUOROBORATE), 50% ON ALUMINA

Page: 4

## 6.4. Reference to other sections

## Section 7: Handling and storage

### 7.1. Precautions for safe handling

**Handling requirements:** Avoid direct contact with the substance. Ensure there is sufficient ventilation of the area.  
Do not handle in a confined space. 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 cool, well ventilated area. Keep container tightly closed.  
**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.

### 8.2. Exposure controls

**Engineering measures:** Ensure there is sufficient ventilation of the area. The floor of the storage room must be impermeable to prevent the escape of liquids.  
**Respiratory protection:** Self-contained breathing apparatus must be available in case of emergency. 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:** Powder  
**Colour:** White to off white  
**Odour:** Odourless  
**Solubility in water:** Partially  
**Melting point/range °C:** 120 (dec.)

### 9.2. Other information

**Other information:** No data available.

## Section 10: Stability and reactivity

[cont...]

## SAFETY DATA SHEET

1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI(TETRAFLUOROBORATE), 50% ON ALUMINA

Page: 5

### 10.1. Reactivity

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

### 10.2. Chemical stability

**Chemical stability:** Stable under normal conditions.

### 10.3. Possibility of hazardous reactions

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

### 10.4. Conditions to avoid

**Conditions to avoid:** Heat. Temperatures > 150 C

### 10.5. Incompatible materials

**Materials to avoid:** Sodium nitrate. Vinyl compounds. Ethylene oxide. Chlorine trifluoride. Halogenated hydrocarbon

### 10.6. Hazardous decomposition products

**Haz. decomp. products:** In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NOx). Hydrogen cyanide (HCN). Hydrogen fluoride (HF). Boron Oxides Aluminium oxides.

## Section 11: Toxicological information

### 11.1. Information on toxicological effects

#### Toxicity values:

Route	Species	Test	Value	Units
ORAL	RAT	LD50	676	mg/kg
DERMAL	RAT	LD50	>2000	mg/kg

#### Relevant hazards for substance:

Hazard	Route	Basis
Serious eye damage/irritation	OPT	Based on test data
Respiratory/skin sensitisation	DRM	Based on test data
STOT-repeated exposure	-	Based on test data

### Symptoms / routes of exposure

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

**Eye contact:** There may be irritation and redness. The eyes may water profusely. Eye-Rabbit-Severe eye irritation -24h

**Ingestion:** There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

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

**Delayed / immediate effects:** No data available.

[cont...]

## SAFETY DATA SHEET

1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI(TETRAFLUOROBORATE), 50% ON ALUMINA

Page: 6

Other information: Not applicable.

### 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.

#### 12.4. Mobility in soil

Mobility: No data available.

#### 12.5. Results of PBT and vPvB assessment

PBT identification: This substance is not identified as a PBT substance.

#### 12.6. Other adverse effects

Other adverse effects: Toxic to aquatic organisms. Water hazard class 1(self-assessment): slightly hazardous for water  
Poisonous for fish and plankton in water bodies

### 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: UN3077

#### 14.2. UN proper shipping name

Shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.  
(1-Fluoro-4-hydroxy-1,4-diazoniabicyclo[2.2.2]octane bis(tetrafluoroborate), 50% on alumina)

#### 14.3. Transport hazard class(es)

Transport class: 9

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## SAFETY DATA SHEET

1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI(TETRAFLUOROBORATE), 50% ON ALUMINA

Page: 7

### 14.4. Packing group

Packing group: III

### 14.5. Environmental hazards

Environmentally hazardous: Yes

Marine pollutant: No

### 14.6. Special precautions for user

Tunnel code: E

Transport category: 3

## Section 15: Regulatory information

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

### 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?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 3:** H318: Causes serious eye damage.  
H373: May cause damage to organs <or state all organs affected, if known> through prolonged or repeated exposure <state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard>.  
H410: Very toxic to aquatic life with long lasting effects.  
R41: Risk of serious damage to eyes.  
R43: May cause sensitisation by skin contact.  
R48/22: Harmful: danger of serious damage to health by prolonged exposure if swallowed.  
R50/53: Very toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

**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

[cont...]

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1-FLUORO-4-HYDROXY-1,4-DIAZONIABICYCLO[2.2.2]OCTANE DI(TETRAFLUOROBORATE), 50% ON ALUMINA

Page: 8

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.