SIGMA-ALDRICH

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SAFETY DATA SHEET

Version 3.12 Revision Date 09/14/2017 Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

1.1	Product identifiers Product name	O-(6-Chlorobenzotriazol-1-yl)-N,N,N',N'-		
		tetramethyluronium hexafluorophosphate		
	Product Number Brand	: 04936 : Sigma-Aldrich		
	CAS-No.	: 330645-87-9		
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 3050 Spruce Street SAINT LOUIS MO 63103 USA		
	Telephone	: +1 800-325-5832		
	Fax	: +1 800-325-5052		
1.4	Emergency telephone number			
	Emergency Phone #	: +1-703-527-3887 (CHEMTREC)		
2. F	AZARDS IDENTIFICATION			

2.1 Classification of the substance or mixture

Not a hazardous substance or mixture.

2.2 GHS Label elements, including precautionary statements

Not a hazardous substance or mixture.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1	Synonyms	 N,N,N',N'-Tetramethyl-O-(6-chloro-1<i>H-benzotriazol-1-yl)uronium hexafluorophosphate 1-[Bis(dimethylamino)methylen]-5-chlorobenzotriazolium 3-oxide hexafluorophosphate HCTU</i> 	l
	Formula	: C ₁₁ H ₁₅ CIF ₆ N ₅ OP	
	Molecular weight	: 413.69 g/mol	
	CAS-No.	: 330645-87-9	

No components need to be disclosed according to the applicable regulations.

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Hydrofluoric (HF) acid burns require immediate and specialized first aid and medical treatment. Symptoms may be delayed up to 24 hours depending on the concentration of HF. After decontamination with water, further damage can occur due to penetration/absorption of the fluoride ion. Treatment should be directed toward binding the fluoride ion as well as the effects of exposure. Skin exposures can be treated with a 2.5% calcium gluconate gel repeated until burning ceases. More serious skin exposures may require subcutaneous calcium gluconate except for digital areas unless the physician is experienced in this technique, due to the potential for tissue injury from increased pressure. Absorption can readily occur through the subungual areas and should be considered when undergoing decontamination. Prevention of absorption of the fluoride ion in cases of ingestion can be obtained by giving milk, chewable calcium carbonate tablets or Milk of Magnesia to conscious victims. Conditions such as hypocalcemia, hypomagnesemia and cardiac arrhythmias should be monitored for, since they can occur after exposure.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration.

In case of skin contact

Wash off with soap and plenty of water. First treatment with calcium gluconate paste.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water.

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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information No data available

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures Avoid dust formation. Avoid breathing vapours, mist or gas. For personal protection see section 8.

6.2 Environmental precautions No special environmental precautions required.

6.3 Methods and materials for containment and cleaning up Sweep up and shovel. Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs. Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place.

Store under inert gas. Keep in a dry place.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters Contains no substances with occupational exposure limit values.

8.2 Exposure controls

Appropriate engineering controls

General industrial hygiene practice.

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).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact Material: Nitrile rubber Minimum layer thickness: 0.11 mm Break through time: 480 min Material tested:Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

No special environmental precautions required.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

	a)	Appearance	Form: powder Colour: white		
	b)	Odour	No data available		
	c)	Odour Threshold	No data available		
	d)	рН	No data available		
	e)	Melting point/freezing point	Melting point/range: 185 - 190 °C (365 - 374 °F)		
	f)	Initial boiling point and boiling range	No data available		
	g)	Flash point	No data available		
	h)	Evaporation rate	No data available		
	i)	Flammability (solid, gas)	No data available		
	j)	Upper/lower flammability or explosive limits	No data available		
	k)	Vapour pressure	No data available		
	I)	Vapour 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)	Auto-ignition 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		
Other safety information					
		Solubility in other solvents	Dimethylformamide		

10. STABILITY AND REACTIVITY

10.1 Reactivity

9.2

No data available

- **10.2 Chemical stability** Stable under recommended storage conditions.
- **10.3** Possibility of hazardous reactions No data available
- **10.4 Conditions to avoid** No data available
- **10.5** Incompatible materials Strong oxidizing agents

10.6 Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx), Oxides of phosphorus, Hydrogen chloride gas, Hydrogen fluoride Other decomposition products - No data available In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - > 200 mg/kg

Inhalation: No data available

Dermal: No data available

No data available

Skin corrosion/irritation No data available

Serious eye damage/eye irritation No data available

Respiratory or skin sensitisation No data available

Germ cell mutagenicity No data available

Carcinogenicity

- IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure No data available

Specific target organ toxicity - repeated exposure No data available

Aspiration hazard No data available

Additional Information

RTECS: Not available

Fluoride ion can reduce serum calcium levels possibly causing fatal hypocalcemia.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

No data available

12.2 Persistence and degradability No data available

12.3 Bioaccumulative potential

No data available

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

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging

Dispose of as unused product.

14. TRANSPORT INFORMATION

DOT (US)

Not dangerous goods

IMDG

Not dangerous goods

ΙΑΤΑ

Not dangerous goods

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

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

No SARA Hazards

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know Components

O-(6-Chlorobenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate	CAS-No. 330645-87-9	Revision Date
New Jersey Right To Know Components		
O-(6-Chlorobenzotriazol-1-yl)-N,N,N',N'-tetramethyluronium hexafluorophosphate	CAS-No. 330645-87-9	Revision Date

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

- HMIS Rating Health hazard:

0

Chronic Health Hazard: Flammability: Physical Hazard	0 0
NFPA Rating	
Health hazard:	0
Fire Hazard:	0
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation Product Safety – Americas Region 1-800-521-8956

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