

SAFETY DATA SHEET

Prepared by: Benedikt Wanner
Date: November 28th, 2017
Version: 0001



Section 1 – Product and Company Identification

- 1.1 Product name:** Synple Chem reagent cartridge 7-Br-9-OMe-Benzoxazepane
1.2 Product code: H091
1.3 Recommended Use: Laboratory chemical consumable
1.4 Company Name: Synple Chem AG,
Vladimir-Prelog-Weg 3,
CH-8093 Zürich,
Switzerland
- 1.5 Contact Details:** Telephone: +41 (0)44 633 42 95
8:00 a.m. – 5:00 p.m. CET
email: info@synplechem.com

Section 2 – Hazards Identification

2.1 Classification of the substance or mixture

Labeling according to Regulation (EC) No 1272/2008

Polymer bound tin reagents

Acute toxicity, Oral (Category 3), H301
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315
Eye irritation (Category 2), H319
Specific target organ toxicity - repeated exposure (Category 1), H372
Acute aquatic toxicity (Category 1), H400
Chronic aquatic toxicity (Category 1), H410

Copper(II) trifluoromethanesulfonate

Skin corrosion (Category 1B), H314

2,6-Lutidine salt

Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Eye irritation (Category 2), H319

2.2 Label elements

Labelling according to Regulation (EC) No 1272/2008

Polymer bound tin reagents

Pictogram



Signal word

Danger

Hazard statement(s)

H301

Toxic if swallowed.

H312

Harmful in contact with skin.

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H315	Causes skin irritation.
H319	Causes serious eye irritation.
H372	Causes damage to organs through prolonged or repeated exposure.
H410	Very toxic to aquatic life with long lasting effects
Precautionary statement(s)	
P272	Avoid release to the environment
P280	Wear protective gloves/ protective clothing
P301 + P310	IF SWALLOWED: Immediately call a poison center or doctor/ physician
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P314	Get medical advice/ attention if you feel unwell
P501	Dispose of contents/ container to an approved waste disposal plant.
Supplemental Hazard Statement(s)	none

Copper(II) trifluoromethanesulfonate

Pictogram



Signal word

Danger

Hazard statement(s)
H314

Causes severe skin burns and eye damage.

Precautionary statement(s)
P280
P305 + P351 + P338

Wear protective gloves/ protective clothing
IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard Statement(s)

none

2,6-Lutidine salt

Pictogram



Signal word

Warning

Hazard statement(s)
H302
H315

Harmful if swallowed.
Causes skin irritation.

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H319

Causes serious eye irritation.

Precautionary statement(s)

P301 + P312 + P330

IF SWALLOWED: Call poison center/ doctor if you feel unwell.
Rinse mouth.

P305 + P351 + P338

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

Supplemental Hazard
Statement(s)

none

2.3 Other hazards

A component of this product is considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB).

Section 3 – Composition / Information on Ingredients

Name:	Polymer bound tin reagent		
Synonyms	–		
Formula	–		
Molecular Weight	–		
Classification	H301, H312, H315, H319, H372, H410, P273, P280, P301 + P310, P305 + P351 + P338, P314, P501		
CAS – No.	EC – No.	Index – No.	Concentration
–	–	–	–

Name:	Copper(II) trifluoromethanesulfonate		
Synonyms	PolyCopper(II) triflate Trifluoromethanesulfonic acid; copper(II) salt Cupric trifluoromethanesulfonate		
Formula	C ₂ CuF ₆ O ₆ S ₂		
Molecular Weight	361.68 g/mol		
Classification	Skin Corr. 1B; H314		
CAS – No.	EC – No.	Index – No.	Concentration
34946-82-2	252-300-8	–	–

Name:	2,6-Lutidine salt		
Synonyms	2,6-Dimethylpyridine salt		
Formula	C ₇ H ₉ N		
Molecular Weight	107.15 g/mol		
Classification	Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2; H302, H315, H319		
CAS – No.	EC – No.	Index – No.	Concentration
108-48-5	203-587-3	–	–

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Name:		Silica gel	
Synonyms		Silica	
Formula		SiO ₂	
Molecular Weight		–	
Classification		–	
CAS – No.	EC – No.	Index – No.	Concentration
112926-00-8	231-545-4	–	–

Name:		SCX-2	
Synonyms		Propylsulfonic acid – functionalized silica gel	
Formula		–	
Molecular Weight		–	
Classification		–	
CAS – No.	EC – No.	Index – No.	Concentration
–	–	–	–

Section 4 – First Aid Measures

4.1 Inhalation

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

4.2 Skin contact

Wash with soap and water

4.3 Eye contact

Wash thoroughly with plenty of water for at least 15 minutes, separating the eyelids with the fingers. If eye irritation persists, seek medical attention

4.4 Ingestion

Wash mouth with plenty of water if person is conscious. Never give anything by mouth to an unconscious person. Consult a physician.

Section 5 – Fire-Fighting Measure

5.1 Suitable Extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide

5.2 Special hazards arising from the cartridge substances or mixtures

May release toxic or flammable vapors during a fire

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Section 6 – Accidental Release Measures

6.1 Personal precautions

In case of a damaged cartridge or leaking reagent out of the cartridge avoid breathing dust. Ventilate the area thoroughly and shut off sources of ignition. Avoid raising dust. Use protective equipment described in Section 8.

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6.2 Environmental precautions

Do not let the materials inside the cartridge enter the drain. Discharge into the environment must be avoided

6.3 Methods and materials for containment and cleaning up

Contain spilled cartridge material and pick up without creating dust. Keep in suitable, closed containers for disposal. For disposal see Section 13.

Section 7– Handling and Storage

7.1 Precautions for safe handling

Do not try to open the reagent cartridge.

7.2 Conditions for safe storage

Keep cartridge in sealed closed bag. Store below 8°C, out of direct sunlight and away from incompatible substances.

7.3 Specific end-usage

Use only in the application the cartridge intended for. Only use with Synple Chem synthesizer devices.

Section 8 – Exposure Controls / Personal Protection

8.1 Personal protective equipment

Respiratory protection

Respiratory protection is not required when materials are contained in the cartridge. When spilled see Section 6.

Hand protection

Handle with gloves. The selected protective gloves have to satisfy the specifications of the EU Directive 89 / 686 / EEC and the standard EN 374 derived from it. Gloves must be inspected prior to use. Use proper glove removal technique (without touching the outer surface of the glove) to avoid skin contact with the product. Dispose of gloves after use in accordance with applicable regulations and good laboratory practice. Wash and dry hands.

Eye protection

Safety glasses with side – shields conforming to EN 166. Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166 (EU).

Skin and body protection

Choose body protection according with good laboratory practices and to specific workplace.

Hygiene measure

Handle in accordance with good laboratory hygiene and safe practice. Wash hands before breaks and at the end of the workday.

Section 9 – Physical and Chemical Properties

9.1 Appearance

Form: Plastic Reagent Cartridge

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Colour: Filled with solid reagents / powder
White / Brown

9.2 Safety Data

pH	No data available
Melting point	No data available
Boiling point	No data available
Flash point	No data available
Ignition temperature	No data available
Lower explosion limit	No data available
Upper explosion limit	No data available
Water solubility	Insoluble

Section 10 – Stability and Reactivity

10.1 Chemical Stability

Stable under recommended storage conditions for at least 1 year

10.2 Conditions to avoid

Avoid temperatures above 60°C, long exposure to air and moisture

10.3 Materials to avoid

Strong oxidizing agents or corrosive chemicals

10.4 Hazardous decomposition products

Hazardous decomposition products formed under hydrolyzing conditions (organic tin species) or fire conditions

Section 11 – Toxicological Information

11.1 Acute Toxicity

Lutidine:

LD50 Oral – Rat – 400 mg/kg

LD 50 Dermal – Guinea pig – 2.500 mg/kg

Other components:

No data available

11.2 Skin corrosion / irritation

No data available

11.3 Serious eye damage / eye irritation

No data available

11.4 Respiratory or skin sensation

No data available

11.5 Germ cell mutagenicity

No data available

11.6 Carcinogenicity

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This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NPT or EPA classification

11.7 Reproductive toxicity

No data available

11.8 Specific target organ toxicity – single exposure

No data available

11.9 Specific target organ toxicity – repeated exposure

No data available

11.10 Aspiration hazard

No data available

11.11 Additional information

Polymer bound tin compounds:

RTECS: Not available

To the best of our knowledge, the chemical, physical and toxicological properties have not been thoroughly investigated.

Silica:

RTECS: VV7315000

Amorphous silica is not classifiable as to its carcinogenicity to humans (Group 3); however, crystalline silica inhaled in the form of quartz or cristobalite from occupational sources is carcinogenic to humans (Group 1, IARC). Therefore, amorphous silica should be handled as if possessing the same hazards as the crystalline form., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Copper(II) Triflate:

RTECS: Not available

Symptoms of systemic copper poisoning may include: capillary damage, headache, cold sweat, weak pulse, and kidney and liver damage, central nervous system excitation followed by depression, jaundice, convulsions, paralysis, and coma. Death may occur from shock or renal failure. Chronic copper poisoning is typified by hepatic cirrhosis, brain damage and demyelination, kidney defects, and copper deposition in the cornea as exemplified by humans with Wilson's disease. It has also been reported that copper poisoning has lead to hemolytic anemia and accelerates arteriosclerosis., Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache

2,6-Lutidine:

RTECS: OK97500000

Cough, Difficulty in breathing, Gastrointestinal disturbance, Ataxia., Unconsciousness, Weakness, Diarrhoea. To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Section 12 – Ecological Information

12.1 Toxicity

No data available

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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

Organic tin species: This substance/mixture contains components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB).

12.6 Other adverse effects

Organic tin species: Very toxic to aquatic life with long lasting effects

Section 13 – Disposal Considerations

13.1 Product (Reagent cartridge)

Contact a licensed professional waste disposal service to dispose of this material. Combine the cartridge with a combustible solvent and burn in a chemical incinerator quipped with an afterburner and scrubber.

13.2 Contaminated packaging

In case some chemical material will exit the cartridge and contaminate the outer packaging dispose the packaging in the same way as the cartridge.

13.3 Un-Contaminated Packaging

Can be disposed with regular waste

Section 14 – Transport Information

14.1 UN number

ADR/RID: 3261

IMDG: 3261

IATA: 3261

14.2 UN proper shipping name

ADR/RID: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (Copper(II) trifluoromethanesulphonate)

IMDG: CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (Copper(II) trifluoromethanesulphonate)

IATA: Corrosive solid, acidic, organic, n.o.s. (Copper(II) trifluoromethanesulphonate)

14.3 Transport hazard class(es)

ADR/RID: 8

IMDG: 8

IATA: 8

14.4 Packaging group

ADR/RID: III

IMDG: III

IATA: III

14.5 Environmental hazards

ADR/RID: yes

IMDG Marine pollutant: yes

IATA: no

14.6 Special precautions for user

No data available

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Section 15 – Regulatory Information

- 15.1 Safety, health and environmental regulations/legislation specific for the substrate or mixture**
No data available
- 15.2 Chemical safety assessment**
For this product a chemical safety assessment was not carried out.

Section 16 – Other Information

This product must only be handled by, or under close supervision of those qualified in the handling and use of potentially hazardous substances. This Safety Data Sheet is offered without charge to the clients of Synple Chem and it is issued only as a guide for safe handling, use, storage, disposal and release. Information contained on this sheet is the most current available to Synple Chem at the time of preparation but does not purport to be all inclusive or a guarantee as to the properties of the product supplied. Synple Chem makes no warranties or representations as to the accuracy and completeness of the information contained herein. Synple Chem shall not be held responsible for the suitability of this information for the user's intended purposes or the consequence of such use, and shall not be liable for any damage or loss, howsoever arising, direct or otherwise.