Safety Data Sheet

1. Identification of the Substance/Mixture and the Supplier

Supplier: National Institute of Advanced Industrial Science and Technology (AIST)
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Identity of Substance/Mixture: Certified reference material: NMIJ CRM 4602-a
1,4-Bis(trimethylsilyl)-2,3,5,6-tetrafluorobenzene for Quantitative NMR (1H, 19F)

Recommended Use of the Chemical and Restriction on Use:
This CRM is intended for use in the calibration of 1H and 19F signal intensity by nuclear magnetic resonance (NMR) spectroscopy. It is also intended for controlling the precision of analysis and confirming the validity of the analytical methods. Do not use this reference material for other purposes than testing/research.

2. Hazards Identification

GHS Classification
- Skin corrosivity/irritant: Class 2
- Severe eye damages/eye irritant: Class 2A
- Respiratory organ sensitization: Hazard Category 1
- Specific target organ toxicity/Systemic toxicity (Single exposure): Class 3 (May cause respiratory irritation)
- Specific target organ toxicity/Systemic toxicity (Repeated exposure): No data

GHS Label Element

Signal Word: Danger
Other Hazards Statement: -
Precautionary Statement: Do not breathe dust, mist, vapors, etc.
Wash skin thoroughly after handling.
Use only outdoor or in a well-ventilated area.
Wear protective gloves/protective clothing/eye protector/face protection.

[Action]
If on skin: Wash with plenty of soap and water.
If inhaled: Remove person to fresh air and keep comfortable for breathing.
If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Call a POISON CENTER or doctor if you feel unwell.
If skin irritation occurs: Get medical advice/attention.
If eyes irritation persists: Get medical advice/attention.
Take off contaminated clothing and wash it before use.

[Storage]
This CRM should be kept at a temperature between 2 °C and 10 °C and shielded from light in a clean place.

[Disposal]
Dispose of this reference material in accordance with applicable legislation and local government ordinance.
Entrust disposal of this reference material to a professional waste disposal company licensed by prefectural governor.

The other hazards than the above do not result in classification or are not classifiable.

3. Composition/Information on Ingredients
Substance or mixture          :  Substance
Chemical name                :  1,4-Bis(trimethylsilyl)-2,3,5,6-tetrafluorobenzene
Synonym                      :  -
Chemical formula             :  -
Molecular weight             :  294.44
CAS number                   :  16956-91-5
Content                      :  Over 99.9 %
Reference Number in Gazetted List in Japan : Act on the Evaluation of Chemical Substances and Regulation of Their Manufacture, etc.
Reference Number in Gazetted List in Japan : Industrial Safety and Health Act

4. First-aid Measures
If in Eyes                    :  Rinse cautiously under running water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get medical advice/attention immediately.
If on Skin                    :  Remove/Take off contaminated clothing, etc. Rinse thoroughly with clean water. Wash polluted clothing, if reuse them.
If Inhaled: Remove victim to fresh air and keep at rest and warm. Then get medical advice/attention immediately.

If Ingested: Rinse mouth thoroughly with water. Do not induce vomiting, if it is not the instructions from a doctor. Get medical advice/attention when feeling unwell.

Predicted immediate and delayed symptoms:
- Cause skin irritation.
- Cause serious eye irritation.
- May cause respiratory irritation.

Protecting Personnel in emergency measures:
- Wear protective equipment such as rubber gloves, eye protective goggles if required.

5. Fire-fighting Measures

Extinguishing Media:
- Alcohol resistant foam.
- Carbon dioxide.
- Dry powder.
- Water spray.
- Use extinguishing media appropriate for surrounding fire.

Fire-Specific Hazards:

Specific Fire-Fighting Method:
- Eliminate ignition sources at the origin of a fire and put out fire by using extinguishing media. Remove movable containers promptly to a safe place.

Protection of Fire-Fighters:
- Use personal protective equipment such as fire protection clothing,
  heat-resistant clothing, protective clothing, breathing apparatus,
  circulating oxygen respirator, rubber gloves, and rubber boots.

6. Accidental Release Measures

Personal Precaution:
- Evacuate unnecessary personnel. Ensure adequate air ventilation.
- Do not breathe dust.

Personal Protective Equipment and Emergency Procedures:
- If an indoor environment, ventilate the affected areas thoroughly until the clean-up operation is completed. Use appropriate personal protective equipment to avoid skin contact and inhalation of dust and gas.

Environmental Precautions:
- Do not allow this CRM to reach sewage systems or any water course.

Recovery and Neutralization:
- Ensure adequate ventilation.
- Stop leak if safe to do so.
- Sweep or shovel spills into appropriate containers for disposal. Minimize generation of dust.
- For disposal of solid materials or residues, refer to section 13: “Disposal considerations”.

Prevention of Secondary Disaster:
- Only qualified personnel equipped with suitable protective equipment may intervene.

7. Handling and Storage
Handling Engineering Precautions: Use appropriate personal protective equipment to avoid inhalation and contact with eyes and skin.
Local and General Ventilation Precautions: Ensure adequate ventilation.
Precautions for Safe Handling: Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe dust, mist, and spray. Wear personal protective equipment. Avoid contact with skin and eyes.
Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

Storage
Appropriate Storage Conditions: This CRM should be kept at a temperature between 2 °C and 10 °C and shielded from light in a clean place.
Store in dry, cool, well-ventilated area.
Store away from oxidizing materials.

Safe Container Packaging Material: Glass

8. Exposure Controls/Personal Protection

Threshold Limit Value
- Not specified

Permissible Concentration (Nitric acid)
- ACGIH: –
- Values recommended by Japan Society for Occupational Health: –
- OSHA PEL TWA: –

Facility engineering
- Ventilation, exhaust: Ensure good ventilation of the work station.
Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.
- Safety: –

Safety management/gas detector
- Storing precaution: This CRM should be kept at a temperature between 2 °C and 10 °C and shielded from light in a clean place.
Store in dry, cool, well-ventilated area.
Store away from oxidizing materials.

Personal Protective equipment
Respiratory protection: Protective gas mask
In case of inadequate ventilation wear respiratory protection.

Hands: Impervious protective gloves

Eyes: Eye protector (Goggle type as necessary)

Skin and Body: Protective clothing (long-sleeved work clothes), protection boots, protective clothing, face mask, etc.

Hygiene measure
Treat in accordance with rules on Industrial hygiene and Industrial safety.

9. Physical and Chemical Properties

- Appearance, etc.: Solid (Powder)
- Color: White
- Odor: No data
- pH: No data
- Melting Point: 53 °C to 55 °C
- Boiling Point: No data
- Flash Point: No data
- Explosive Range: No data
- Vapor Pressure: No data
- Relative vapor density (Air = 1): No data
- Specific Gravity or Bulk Specific Gravity: 1.25 g/cm³ at 25 °C
- Solubility: Soluble in organic solvents such as methanol and acetone.
- n-octanol/water partition coefficient, log Po/w: No data
- Spontaneous ignition temperature: No data
- Decomposition temperature: No data
- Combustibility: No data

10. Stability and Reactivity

Stability: Stable in normal conditions
Reactivity: Decomposition will not occur if used and stored in normal conditions. Reacts with strong oxidizing agents.

Conditions to Avoid: No data
Incompatible material: Strong oxidizing agents
Hazardous Decomposition Products: Carbon monoxide(CO), carbon dioxide(CO₂), hydrogen fluoride(HF) and Silicon oxide(SiO₂)

11. Toxicological Information

Acute Toxicity: Not classified.
Skin Corrosion/Irritation: Causes skin irritation.
Serious Eye Damage/Eye Irritation: Causes serious eye irritation.
Specific Target Organ Toxicity/Systemic Toxicity (Single Exposure): May cause respiratory irritation.
Specific Target Organ Toxicity/Systemic Toxicity (Repeated): Not classified
Exposure)
Aspiration hazard Not classified
※This reference material is stable under the normal condition, however, when handling this
reference material under special conditions such as the use under the high temperature etc. it
is recommended to take safety precautions appropriate to use.

12. Ecological Information

Hazardous to the aquatic environment, short-term (Acute) : No data
Hazardous to the aquatic environment, long-term (Chronic) : No data
Ecotoxicity : No data
Persistence and Degradability : No data
Bioaccumulative Potential : No data
Mobility in soil : No data
Ozone depletion potential : No data

12. Ecological Information

Persistence and Degradability
・ No data
Bioaccumulative Potential
・ No data
Ecotoxicity
・ Crystacea (Daphnia magna): 48 hours EC50=0.492 mg/L

13. Disposal Considerations

Residual Waste : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.
When the above-mentioned treatments are not possible, entrust disposal of residual waste to a professional waste disposal company licensed by prefectural governor.
Contaminated Container and Package : Dispose of containers after thoroughly removing their contents.

14. Transport Information

UN Number : *
UN Classification : *
Material name : *
Container grade : *
Marine pollutant : *
Precautions : Avoid direct sunlight and transfer with care not to spill/leak by dropping or falling, etc.
15. Regulatory Information

◇ No applicable laws and regulations.
Observe general handling precautions on chemicals.

◎ This SDS is originally prepared for the use of the material in Japan, thus the stated laws and regulations are stipulated and carried out in Japan. The use of the material in other countries should be referred to and by application of the relevant laws and regulations of the country in which the material will be used.

16. Other Information

Others
The information in this document is not intended to be exhaustive and is based on currently available information and data. The measures given in this document are applicable only to normal handling conditions. When handling this reference material under special conditions etc., it is recommended to take safety measures appropriate to each specific application and context of use. This document is intended to provide information and not intended to guarantee anything in handling this reference material.