

SAFETY DATA SHEET

Version 8.12
Revision Date 08/08/2025
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Cyclopentadienylhafnium(IV) trichloride
Product Number : 484369
Brand : Aldrich
CAS-No. : 61906-04-5

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

Identified uses : Laboratory chemicals, Synthesis of substances
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES
Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Skin corrosion : Category 1B
Serious eye damage : Category 1

Germ cell mutagenicity	: Category 1B
Carcinogenicity	: Category 1A
Specific target organ toxicity - repeated exposure	: Category 1 (Blood)
Short-term (acute) aquatic hazard	: Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms	:	
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Signal Word	:	Danger
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Hazard Statements	:	H314 Causes severe skin burns and eye damage. H340 May cause genetic defects. H350 May cause cancer. H372 Causes damage to organs (Blood) through prolonged or repeated exposure. H402 Harmful to aquatic life.
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Precautionary statements	:	Prevention: P201 Obtain special instructions before use. P202 Do not handle until all safety precautions have been read and understood. P260 Do not breathe dust. P264 Wash skin thoroughly after handling. P270 Do not eat, drink or smoke when using this product. P273 Avoid release to the environment. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
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Response:

P301 + P330 + P331 IF SWALLOWED:	Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair):	Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P310 IF INHALED:	Remove person to fresh air and keep comfortable for breathing.
Immediately call a POISON CENTER/ doctor.	
P305 + P351 + P338 + P310 IF IN EYES:	Rinse

cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor. P308 + P313 IF exposed or concerned: Get medical advice/ attention.

P363 Wash contaminated clothing before reuse.

Storage:

P405 Store locked up.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Cyclopentadienylhafnium (IV) trichloride	61906-04-5*	>= 90 - <= 100	-
benzene	71-43-2*	>= 5 - < 10	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : First aiders need to protect themselves. Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air. Call in physician.

In case of skin contact : In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact : After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed : After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

Most important : The most important known symptoms and effects are

Aldrich - 484369

Page 3 of 15

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symptoms and effects, both acute and delayed	described in the labelling (see section 2.2) and/or in section 11
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO2) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible. Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	: Carbon oxides Hydrogen chloride gas Hafnium oxide
Specific extinguishing methods	: No data available
Further information	: Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Avoid generation and inhalation of dusts in all circumstances. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	: Do not let product enter drains.
Methods and materials for containment and cleaning up	: Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on safe handling	: Work under hood. Do not inhale substance/mixture.
Further information on storage conditions	: Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.
Storage class	: 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects
Recommended storage temperature	: Recommended storage temperature see product label.
Further information on storage stability	: Handle and store under inert gas. Air sensitive.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
benzene	71-43-2	TWA	0.5 ppm	ACGIH

	STEL	2.5 ppm	ACGIH
	TWA	10 ppm	OSHA Z-2
	CEIL	25 ppm	OSHA Z-2
	Peak	50 ppm	OSHA Z-2
	TWA	0.1 ppm	NIOSH REL
	ST	1 ppm	NIOSH REL

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: Filter type P3

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Hand protection

Material	: Nitrile rubber
Break through time	: 480 min
Glove thickness	: 0.11 mm
Protective index	: Full contact
Manufacturer	: KCL 741 Dermatril® L
Material	: Nitrile rubber
Break through time	: 480 min
Glove thickness	: 0.11 mm
Protective index	: Splash contact
Manufacturer	: KCL 741 Dermatril® L
Remarks	: Handle with impervious gloves. This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Eye protection	: Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles
Skin and body protection	: protective clothing
Hygiene measures	: Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: powder
Color	: tan
Odor	: No data available
Odor Threshold	: No data available
pH	: No data available
Melting point/ range	: 257 °F / 125 °C Method: lit.
Boiling point/boiling range	: No data available
Flash point	: No data available
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapor pressure	: No data available
Relative vapour density	: No data available
Relative density	: No data available

Density	: No data available
Water solubility	: No data available
Partition coefficient: n-octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Molecular weight	: 349.94 g/mol
Particle characteristics	
Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: no information available
Incompatible materials	: Strong oxidizing agents
Hazardous decomposition products	: In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

Acute toxicity estimate Oral - > 5,000 mg/kg
(Calculation method)

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Remarks: No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: 1 - Group 1: Carcinogenic to humans (benzene)

NTP: Known - Known to be human carcinogen (benzene)

OSHA: OSHA specifically regulated carcinogen (benzene)

Reproductive toxicity

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

11.2 Additional Information

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin.

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

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To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (Cyclopentadienylhafnium(IV) trichloride)

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

benzene:

Toxicity to fish : LC50 (Oryzias latipes (Orange-red killifish)): > 100 mg/l
End point: mortality
Exposure time: 96 h
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 203
GLP: yes

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): > 1,000 mg/l
End point: Immobilization
Exposure time: 48 h
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 202
GLP: yes

NOEC (Daphnia magna (Water flea)): > 1,000 mg/l
End point: Immobilization
Exposure time: 48 h
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 202
GLP: yes

Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata (green algae)): > 1,000 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes

NOEC (Pseudokirchneriella subcapitata (green algae)): >= 1,000 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes

Toxicity to fish (Chronic toxicity) : NOEC (Pimephales promelas (fathead minnow)): 0.8 mg/l
Exposure time: 32 d

Test Type: flow-through test
Analytical monitoring: yes
Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : LC50 (Daphnia magna (Water flea)): > 100 mg/l
End point: mortality
Exposure time: 21 d
Test Type: semi-static test
Analytical monitoring: yes
Method: OECD Test Guideline 211
GLP: yes

Toxicity to microorganisms : EC50 (activated sludge): > 1,000 mg/l
Exposure time: 3 h
Test Type: static test
Method: OECD Test Guideline 209
GLP: yes

Ecotoxicology Assessment

Chronic aquatic toxicity : Harmful to aquatic life with long lasting effects.

Persistence and degradability

Components:

benzene:

Biodegradability : aerobic
Inoculum: activated sludge, non-adapted
Concentration: 17 mg/l
Result: Readily biodegradable.
Biodegradation: 96 %
Exposure time: 28 d
Method: OECD Test Guideline 301F
GLP: yes

Bioaccumulative potential

Components:

benzene:

Bioaccumulation : Species: Leuciscus idus (Golden orfe)
Bioconcentration factor (BCF): 10
Exposure time: 3 d
Concentration: 0.05 mg/l

Partition coefficient: n-octanol/water : log Pow: 2.13 (77 °F / 25 °C)
pH: 7
Remarks: Bioaccumulation is not expected.
(ECHA)

Mobility in soil

No data available

Other adverse effects

Components:

benzene:

Additional ecological information : Endangers drinking-water supplies if allowed to enter soil or water.

Discharge into the environment must be avoided.

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No. : UN 3261
Proper shipping name : Corrosive solid, acidic, organic, n.o.s.
(Cyclopentadienylhafnium(IV) trichloride)
Class : 8
Packing group : II
Labels : Class 8 - Corrosive substances
Packing instruction (cargo aircraft) : 863
Packing instruction (passenger aircraft) : 859

IMDG-Code

UN number : UN 3261
Proper shipping name : CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S.
(Cyclopentadienylhafnium(IV) trichloride)
Class : 8
Packing group : II
Labels : 8
EmS Code : F-A, S-B
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number	:	UN 3261
Proper shipping name	:	Corrosive solid, acidic, organic, n.o.s. (Cyclopentadienylhafnium(IV) trichloride)
Class	:	8
Packing group	:	II
Labels	:	Class 8 - Corrosive substances
ERG Code	:	154
Marine pollutant	:	no
Poison Inhalation Hazard	:	No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION**CERCLA Reportable Quantity**

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
benzene	71-43-2	10	200
benzene	71-43-2	10	10 (D018)

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard
Chronic Health Hazard

SARA 313 : The following components are subject to reporting levels established by SARA Title III, Section 313:
benzene 71-43-2 >= 5 - < 10 %

US State Regulations**Massachusetts Right To Know**

benzene 71-43-2

Pennsylvania Right To Know

benzene 71-43-2

Maine Chemicals of High Concern

benzene 71-43-2

Vermont Chemicals of High Concern

benzene

71-43-2

Washington Chemicals of High Concern

benzene

71-43-2

California Prop. 65

WARNING: This product can expose you to chemicals including benzene, which is/are known to the State of California to cause cancer and birth defects or other reproductive harm. For more information go to www.P65Warnings.ca.gov.

The components of this product are reported in the following inventories:

TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	: USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	: USA. NIOSH Recommended Exposure Limits
OSHA Z-2	: USA. Occupational Exposure Limits (OSHA) - Table Z-2
ACGIH / TWA	: 8-hour, time-weighted average
ACGIH / STEL	: Short-term exposure limit
NIOSH REL / TWA	: Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek
NIOSH REL / ST	: STEL - 15-minute TWA exposure that should not be exceeded at any time during a workday
OSHA Z-2 / TWA	: 8-hour time weighted average
OSHA Z-2 / CEIL	: Acceptable ceiling concentration
OSHA Z-2 / Peak	: Acceptable maximum peak above the acceptable ceiling concentration for an 8-hr shift

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing

Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Revision Date : 08/08/2025

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Aldrich - 484369

Page 15 of 15

The life science business of Merck KGaA, Darmstadt, Germany
operates as MilliporeSigma in the US and Canada

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