



HEXAFLUOROACETONE TRIDEUTERATE (D, 99%)

Safety Data Sheet

according to Regulation (EC) No. 1907/2006 (REACH) with its amendment Regulation (EU) 2015/830 and according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 29/03/2011

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Supersedes: 10/12/2015

Version: 2.1

DLM-1020

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form	: Substance
Substance name	: HEXAFLUOROACETONE TRIDEUTERATE (D, 99%)
EC-No.	: 211-676-3 (Unlabeled)
CAS-No.	: 109640-39-3
Product code	: DLM-1020
Formula	: CF ₃ COCF ₃ (D ₂ O) ₃
Synonyms	: Hexafluoro-2-propanone deuterate

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

1.2.1. Relevant identified uses

No additional information available

1.2.2. Uses advised against

No additional information available

1.3. Details of the supplier of the safety data sheet

Cambridge Isotope Laboratories, Inc.
50 Frontage Road
Andover, MA 01810
USA

USA: 1-800-322-1174 Int: 1-978-749-8000

cilsales@isotope.com www.isotope.com

Emergency telephone number

Emergency numbers:

Chemtrec: 1-800-424-9300 (24 hours)

International: 1-703-741-5970 (24 hours)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification according to Regulation (EC) No. 1272/2008 [CLP]

Acute Tox. 3 (Oral)	H301
Acute Tox. 1 (Dermal)	H310
Acute Tox. 3 (Inhalation:dust,mist)	H331
Skin Corr. 1A	H314
Eye Dam. 1	H318
Repr. 2	H361fd

Full text of hazard classes and H-statements : see section 16

Classification according to Directive 67/548/EEC [DSD] or 1999/45/EC [DPD]

Repr.Cat.3; R62

R14

T+; R27

Xi; R36

Repr.Cat.3; R63

C; R34

T; R25

T; R23

Xi; R41

Xi; R39

C; R35

Full text of R-phrases: see section 16

GHS-US classification

Acute Tox. 3 (Oral) H301

Acute Tox. 1 (Dermal) H310

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Acute Tox. 3 (Inhalation) H331
Skin Corr. 1A H314
Eye Dam. 1 H318
Repr. 2 H361

Full text of H statements : see section 16

Adverse physicochemical, human health and environmental effects

Liver Kidney, Testes, Thymus.

2.2. Label elements

Labeling according to Regulation (EC) No. 1272/2008 [CLP]

Hazard pictograms (CLP) :



Signal word (CLP) :

Danger

Hazard statements (CLP) :

H301+H331 - Toxic if swallowed or if inhaled
H310 - Fatal in contact with skin
H314 - Causes severe skin burns and eye damage
H361fd - Suspected of damaging fertility. Suspected of damaging the unborn child.

Precautionary statements (CLP) :

P260 - Do not breathe dust, fume, gas, mist, spray, vapors.
P264 - Wash Both hands thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear protective clothing, protective gloves.
P301+P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor.
P301+P330+P331 - IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P302+P352 - IF ON SKIN: Wash with plenty of water.

EUH phrases

: EUH014 - Reacts violently with water

GHS-US labeling

Hazard pictograms (GHS-US) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H301+H331 - Toxic if swallowed or if inhaled
H310 - Fatal in contact with skin
H314 - Causes severe skin burns and eye damage
H318 - Causes serious eye damage
H361 - (Dermal, Inhalation, oral)

Precautionary statements (GHS-US) :

P201 - Obtain special instructions before use.
P202 - Do not handle until all safety precautions have been read and understood.
P260 - Do not breathe dust, fume, gas, mist, spray, vapors.
P261 - Avoid breathing dust, fume, gas, mist, spray, vapors.
P262 - Do not get in eyes, on skin, or on clothing.
P264 - Wash Both hands thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear protective clothing, protective gloves.
P301+P310 - If swallowed: Immediately call a poison center or doctor
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 - If inhaled: Remove person to fresh air and keep comfortable for breathing
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P308+P313 - If exposed or concerned: Get medical advice/attention.
P310 - Immediately call a poison center or doctor
P311 - Call a poison center or doctor
P321 - Specific treatment (see Hazard pictograms (CLP) on this label)
P330 - Rinse mouth.

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P361 - Take off immediately all contaminated clothing.
P363 - Wash contaminated clothing before reuse.
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.
P405 - Store locked up.
P501 - Dispose of contents/container to Comply with applicable regulations

2.3. Other hazards

No additional information available

SECTION 3: Composition/Information on ingredients

3.1. Substances

Name	Product identifier	%	Classification according to Directive 67/548/EEC
HEXAFLUOROACETONE TRIDEUTERATE (D, 99%)	(CAS-No.) 109640-39-3 (EC-No.) 211-676-3 (Unlabeled)	100	Repr.Cat.3; R62 R14 T+; R27 Xi; R36 Repr.Cat.3; R63 C; R34 T; R25 T; R23 Xi; R41 Xi; R39 C; R35

Name	Product identifier	%	Classification according to Regulation (EC) No. 1272/2008 [CLP]
HEXAFLUOROACETONE TRIDEUTERATE (D, 99%)	(CAS-No.) 109640-39-3 (EC-No.) 211-676-3 (Unlabeled)	100	Acute Tox. 3 (Oral), H301 Acute Tox. 1 (Dermal), H310 Acute Tox. 3 (Inhalation:dust,mist), H331 Skin Corr. 1A, H314 Eye Dam. 1, H318 Repr. 2, H361fd

Full text of R- and H- phrases: see section 16

Name	Product identifier	%	GHS-US classification
HEXAFLUOROACETONE TRIDEUTERATE (D, 99%) (Main constituent)	(CAS-No.) 109640-39-3	100	Acute Tox. 3 (Oral), H301 Acute Tox. 1 (Dermal), H310 Acute Tox. 3 (Inhalation), H331 Skin Corr. 1A, H314 Eye Dam. 1, H318 Repr. 2, H361

Full text of H-phrases: see section 16

3.2. Mixtures

Not applicable

SECTION 4: First aid measures

4.1. Description of first aid measures

First-aid measures general	: Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.
First-aid measures after inhalation	: If breathed in, move person to fresh air. If not breathing, give artificial respiration. Consult a physician.
First-aid measures after skin contact	: Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.
First-aid measures after eye contact	: Flush eye with water for 15 minutes. Get medical attention.
First-aid measures after ingestion	: Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

4.2. Most important symptoms and effects, both acute and delayed

Symptoms/effects after inhalation	: Toxic if inhaled. Causes respiratory tract irritation.
Symptoms/effects after skin contact	: Toxic if absorbed through skin. Causes skin irritation.
Symptoms/effects after eye contact	: Causes eye irritation.
Symptoms/effects after ingestion	: Toxic if swallowed.

4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media : In case of fire: Use Carbon dioxide (CO₂) dry powder.

5.2. Special hazards arising from the substance or mixture

Reactivity : Reacts violently with water.

5.3. Advice for firefighters

Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Not flammable or combustible.

6.1.1. For non-emergency personnel

Emergency procedures : Wear respiratory protection. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.

6.1.2. For emergency responders

No additional information available

6.2. Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3. Methods and material for containment and cleaning up

For containment : Soak up with inert absorbent material and dispose of as hazardous waste. Do not flush with water. Keep in suitable, closed containers for disposal.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Additional hazards when processed : Avoid contact with skin and eyes. Avoid inhalation of vapour or mist. Normal measures for preventive fire protection.

Hygiene measures : Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Store at room temperature away from light and moisture.

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

No additional information available

8.2. Exposure controls

Personal protective equipment : Gloves. Protective clothing. Protective goggles. Self-contained breathing apparatus.



Eye protection : Wear safety glasses with side shields (or goggles) and a face shield.

Skin and body protection : Complete suit protecting against chemicals, Flame retardant antistatic protective clothing. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection : When appropriate, use NIOSH/CEN approved respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state : Liquid

Appearance : Liquid.

Molecular mass : 226.11 g/mol (Labeled)

Color : Colorless.

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Odor	: No data available.
Odor threshold	: No data available
pH	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Melting point	: 18 - 21 °C (64 - 70 °F) - lit.
Freezing point	: No data available
Boiling point	: 106 - 108 °C (223 - 226 °F) - at 1, 1013 hPa (760 mmHg)
Flash point	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: 14681.6 hPa (11,012.1 mmHg) at 55 °C (131 °F); 6,031.2 hPa (4,523.8 mmHg) at 21 °C (70 °F)
Relative vapor density at 20 °C	: 7.6 - (Air = 1.0)
Relative density	: No data available
Specific gravity / density	: 1.579 g/cm ³ at 25 °C (77 °F)
Solubility	: No data available
Log Pow	: No data available
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Explosion limits	: No data available

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

Reacts violently with water.

10.2. Chemical stability

One year after receipt of order if stored as stated in "Storage" section. Re-QC after one year.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Exposure to moisture.

10.5. Incompatible materials

Strong oxidizing agents, Water.

10.6. Hazardous decomposition products

Formed under fire conditions: Carbon oxides, Hydrogen fluoride.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Oral: Toxic if swallowed. Dermal: Fatal in contact with skin. Inhalation:dust,mist: Toxic if inhaled.

HEXAFLUOROACETONE TRIDEUTERATE (D, 99%) (109640-39-3)	
ATE CLP (oral)	100.000 mg/kg body weight
ATE CLP (dermal)	5.000 mg/kg body weight
ATE CLP (dust, mist)	0.500 mg/l/4h

Skin corrosion/irritation	: Causes severe skin burns and eye damage. No data available
Serious eye damage/irritation	: Causes serious eye damage. No data available
Respiratory or skin sensitization	: Not available No data available
Germ cell mutagenicity	: Not available

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Carcinogenicity	: Not classified
Reproductive toxicity	: Not available
Specific target organ toxicity – single exposure	: Not classified Inhalation - May cause respiratory irritation
Specific target organ toxicity – repeated exposure	: Not classified No data available
Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: Burning sensation. Cough. Wheezing. Laryngitis. Shortness of breath. Headache. Nausea. Vomiting. Dizziness. Central nervous system depression.
Symptoms/effects after inhalation	: Toxic if inhaled. Causes respiratory tract irritation.
Symptoms/effects after skin contact	: Toxic if absorbed through skin. Causes skin irritation.
Symptoms/effects after eye contact	: Causes eye irritation.
Symptoms/effects after ingestion	: Toxic if swallowed.

SECTION 12: Ecological information

12.1. Toxicity

No additional information available

12.2. Persistence and degradability

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Persistence and degradability	Not available.
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12.3. Bioaccumulative potential

HEXAFLUOROACETONE TRIDEUTERATE (D, 99%) (109640-39-3)

Bioaccumulative potential	Not available.
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12.4. Mobility in soil

HEXAFLUOROACETONE TRIDEUTERATE (D, 99%) (109640-39-3)

Ecology - soil	Not available.
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12.5. Results of PBT and vPvB assessment

No additional information available

12.6. Other adverse effects

Other adverse effects : Not available.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

Regional legislation (waste) : Waste materials should be disposed of under conditions which meet Federal, State, and local environmental control regulations.

SECTION 14: Transport information

In accordance with ADR / RID / IMDG / IATA / ADN

14.1. UN number

UN-No.(DOT)	: 2552
DOT NA no.	UN2552

14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Hexafluoroacetone hydrate, liquid
Class (DOT)	: 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132
Hazard labels (DOT)	: 6.1 - Poison



Packing group (DOT) : II - Medium Danger

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DOT Special Provisions (49 CFR 172.102)	: IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized. T7 - 4 178.274(d)(2) Normal..... 178.275(d)(3) TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where: tr is the maximum mean bulk temperature during transport, tf is the temperature in degrees celsius of the liquid during filling, and a is the mean coefficient of cubical expansion of the liquid between the mean temperature of the liquid during filling (tf) and the maximum mean bulk temperature during transportation (tr) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where: d15 and d50 are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.
DOT Packaging Exceptions (49 CFR 173.xxx)	: 153
DOT Packaging Non Bulk (49 CFR 173.xxx)	: 202
DOT Packaging Bulk (49 CFR 173.xxx)	: 243
Marine pollutant	: No

14.3. Additional information

Other information : No supplementary information available.

Overland transport

Packing group (ADR)	: II
Class (ADR)	: 6.1 - Toxic substances
Hazard identification number (Kemler No.)	: 60
Classification code (ADR)	: T1
Hazard labels (ADR)	: 6.1 - Toxic substances



Orange plates	: An orange rectangular plate with a black border, containing the number 60 in the top half and 2552 in the bottom half.
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Tunnel restriction code (ADR)	: D/E
Limited quantities (ADR)	: 100ml
EAC	: 2X
Excepted quantities (ADR)	: E4

Transport by sea

DOT Vessel Stowage Location	: B - (i) The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) "On deck only" on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.
DOT Vessel Stowage Other	: 40 - Stow "clear of living quarters"
MFAG-No	: 151

Air transport

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: 5 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	: 60 L
Civil Aeronautics Law	: Toxic and infectious substances/Toxic substances

14.4. Environmental hazards

Other information : No supplementary information available.

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14.5. Special precautions for user

14.6. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

SECTION 15: Regulatory information

15.1. US Federal regulations

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SARA Section 311/312 Hazard Classes	Immediate (acute) health hazard Delayed (chronic) health hazard
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15.2. International regulations

CANADA

No additional information available

15.2.1. National regulations

No additional information available

15.3. US State regulations

HEXAFLUOROACETONE TRIDEUTERATE (D, 99%)(109640-39-3)

U.S. - California - Proposition 65 - Carcinogens List	No
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
State or local regulations	U.S. - Pennsylvania - RTK (Right to Know) List U.S. - New Jersey - Right to Know Hazardous Substance List WARNING! This product contains a chemical known by the state of California to cause birth defects or other reproductive harm.

SECTION 16: Other information

Other information : This product is not radioactive. The data given for this product are those of the corresponding unlabeled compound, unless specifically indicated otherwise. Health and safety data for labeled compounds are generally not available, but are assumed to be similar or identical to the corresponding unlabeled compound.

Full text of R-, H- and EUH-phrases:

Acute Tox. 1 (Dermal)	Acute toxicity (dermal) Category 1
Acute Tox. 3 (Inhalation:dust,mist)	Acute toxicity (inhalation:dust,mist) Category 3
Acute Tox. 3 (Oral)	Acute toxicity (oral) Category 3
Eye Dam. 1	Serious eye damage/eye irritation Category 1
Repr. 2	Reproductive toxicity Category 2
Skin Corr. 1A	Skin corrosion/irritation Category 1A
H301	Toxic if swallowed
H310	Fatal in contact with skin
H314	Causes severe skin burns and eye damage
H318	Causes serious eye damage
H331	Toxic if inhaled
H361fd	Suspected of damaging fertility. Suspected of damaging the unborn child.
EUH014	Reacts violently with water
R14	Reacts violently with water
R23	Toxic by inhalation
R25	Toxic if swallowed
R27	Very toxic in contact with skin
R34	Causes burns
R35	Causes severe burns
R36	Irritating to eyes

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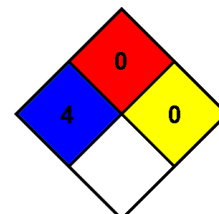
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R39	Danger of very serious irreversible effects
R41	Risk of serious damage to eyes
R62	Possible risk of impaired fertility
R63	Possible risk of harm to the unborn child
C	Corrosive
T	Toxic
T+	Very toxic
Xi	Irritant

- NFPA health hazard : 4 - Materials that, under emergency conditions, can be lethal.
- NFPA fire hazard : 0 - Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.
- NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

- Health : 2 Moderate Hazard - Temporary or minor injury may occur
- Flammability : 0 Minimal Hazard
- Physical : 0 Minimal Hazard

CIL Substance SDS

This information is based on our current knowledge and is intended to describe the product for the purposes of health, safety and environmental requirements only. It should not therefore be construed as guaranteeing any specific property of the product