Hexafluoroacetone trihydrate

sc-250103

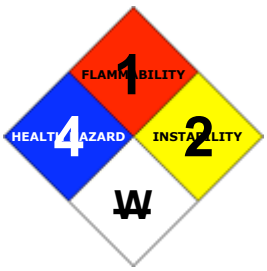
Material Safety Data Sheet

Hazard Alert Code Key:	EXTREME	HIGH	MODERATE	LOW

Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME
Hexafluoroacetone trihydrate

STATEMENT OF HAZARDOUS NATURE
CONSIDERED A HAZARDOUS SUBSTANCE ACCORDING TO OSHA 29 CFR 1910.1200.

NFPA


SUPPLIER
Santa Cruz Biotechnology, Inc.
2145 Delaware Avenue
Santa Cruz, California 95060
800.457.3801 or 831.457.3800
EMERGENCY:
ChemWatch
Within the US & Canada: 877-715-9305
Outside the US & Canada: +800 2436 2255
(1-800-CHEMCALL) or call +613 9573 3112

PRODUCT USE
Used in chemical synthesis. Solvent for insoluble Acetal / Polyamide resins. Degradation product of HFC-227ea

SYNONYMS
C3F6O, F3CCOCF3, "C3F6O. 1.5H2O.", "F3CCOCF3. 1.5H2O.", "acetone, hexafluoro", "1, 1, 1, 3, 3, 3-hexafluoroacetone sesquihydrate", hydrates, "1, 1, 1, 3, 3, 3-hexafluoroacetone trihydrate", "C3F6O. 3H2O.", "F3CCOCF3. 3H2O.", "1, 1, 1, 3, 3, 3-hexafluoroacetone dihydrate", "C3F6O. 2H2O.", "F3CCOCF3. 2H2O.", "1, 1, 1, 3, 3, 3-hexafluoroacetone monohydrate", "C3F6O. H2O.", "F3CCOCF3. H2O."

Section 2 - HAZARDS IDENTIFICATION

CHEMWATCH HAZARD RATINGS

		Min	Max
Flammability:	1		
Toxicity:	3		
Body Contact:	3		
Reactivity:	2		
Chronic:	3		

Min/Nil=0
Low=1
Moderate=2
High=3
Extreme=4

CANADIAN WHMIS SYMBOLS

EMERGENCY OVERVIEW

RISK

Causes burns.
Risk of serious damage to eyes.
May impair fertility.
Possible risk of harm to the unborn child.
Toxic in contact with skin and if swallowed.
Risk of explosion if heated under confinement.

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

■ Toxic effects may result from the accidental ingestion of the material; animal experiments indicate that ingestion of less than 40 gram may be fatal or may produce serious damage to the health of the individual.
■ The material can produce chemical burns within the oral cavity and gastrointestinal tract following ingestion.
■ After oral dosing of hexafluoroacetone in rats, moderate to severe CNS depression persisting for several days was noted. No other signs were discernible. On gross necropsy, no abnormalities were evident.

EYE

■ The material can produce chemical burns to the eye following direct contact. Vapors or mists may be extremely irritating.
■ If applied to the eyes, this material causes severe eye damage.
■ Undiluted hexafluoroacetone sesquihydrate was instantly painful and produced a severe extensive injury in the rabbit eye. When rinsed with water 20 seconds after instillation, the eye appeared to return to normal 29 days after exposure except for a small corneal injury with local vascularisation. The unwashed eye showed extensive corneal opacity, scar tissue, pannus, and chronic conjunctivitis.

SKIN

■ Skin contact with the material may produce toxic effects; systemic effectsmay result following absorption.
■ The material can produce chemical burns following direct contactwith the skin.
■ Undiluted hexafluoroacetone sesquihydrate is a severe skin irritant as expected by its acidic (pH = 1) nature. Concentrations below 50% produced mild to no irritation on rabbit skin. The irritation response at higher concentrations included definite erythema that became scaly and developed crusts 1 to 5 days postapplication. One drop of undiluted dihydrate produced marked erythema and blanching to guinea pig skin, but no irritation was seen with dilutions of 0.1 to 10%.
After dermal application, there was no measurable amount of material remaining on the skin of the rabbits at the end of the exposure period. The exposed area was erythematous and scaly and developed crusts (eschar formation) 2 to 5 days after exposure. Mild CNS depression preceded death, but no other abnormal signs were evident. On gross necropsy, no abnormalities were present except for discolouration and oedema of the exposed skin.
■ Fluorides are easily absorbed through the skin and cause death of soft tissue and erode bone. Healing is delayed and death of tissue may continue to spread beneath skin.
■ Open cuts, abraded or irritated skin should not be exposed to this material.
■ Solution of material in moisture on the skin, or perspiration, may markedly increase skin corrosion and accelerate tissue destruction.
■ Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

■ If inhaled, this material can irritate the throat andlungs of some persons.
■ The material is not thought to produce adverse health effects following inhalation (as classified using animal models). Nevertheless, adverse effects have been produced following exposure of animals by at least one other route and good hygiene practice requires that exposure be kept to a minimum and that suitable control measures be used in an occupational setting.
■ Symptoms of exposure may be burning sensation, coughing, wheezing, shortness of breath, headache, nausea, vomiting. An acute severe inhalation exposure may be fatal as a result of spasm, inflammation and edema of larynx, chemical pneumonitis and pulmonary oedema.
For hexafluoroacetone dihydrate, the maximum concentration causing irritation of the upper respiratory tract was reported to be 32 mg/m3 (equivalent to 26 mg/m3 hexafluoroacetone).
After inhalation exposure by rats, depression of the central nervous system (CNS) was manifest as hind leg instability and loss of postural and righting reflexes . The effects persisted for several hours. Most of the fatalities occurred 2 to 6 days after exposure. There was little, if any, lung damage. There were no
histological findings in heart, kidney, or liver.
■ Acute effects of fluoride inhalation include irritation of nose and throat, coughing and chest discomfort. A single acute over-exposure may even cause nose bleed.
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CHRONIC HEALTH EFFECTS

■ Repeated or prolonged exposure to corrosives may result in the erosion of teeth, inflammatory and ulcerative changes in the mouth and necrosis (rarely) of the jaw. Bronchial irritation, with cough, and frequent attacks of bronchial pneumonia may ensue.
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Ample evidence exists from experimentation that reduced human fertility is directly caused by exposure to the material.
Results in experiments suggest that this material may cause disorders in the development of the embryo or fetus, even when no signs of poisoning show in the mother.
Limited evidence suggests that repeated or long-term occupational exposure may produce cumulative health effects involving organs or

biochemical systems.
Animal testing with the gas at 12 ppm for rats and dogs (13 weeks @ 6 hour) showed testicular degeneration and atrophy, hyperglycaemia, anemia.
In reproduction toxicity studies in which pregnant rats were exposed during organogenesis, minimal but statistically significant decreases in female offspring body weight were seen at exposure by inhalation to 0.76 mg/m3, and a higher incidence of hydronephrosis, one anophthalmic foetus and 2 stunted fetuses at a dermal dose of 0.75 mg /kg bw , the lowest concentration/dose tested.
Hydrogen fluoride easily penetrates the skin and causes destruction and corrosion of the bone and underlying tissue. Ingestion causes severe pains and burns in the mouth and throat and blood calcium levels are dangerously reduced.
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Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
hexafluoroacetone hydrate	13098-39-0	>97
as		
hexafluoroacetone	684-16-2	
hydrolysis may yield		
hydrogen fluoride	7664-39-3	

Section 4 - FIRST AID MEASURES

SWALLOWED
· For advice, contact a Poisons Information Center or a doctor at once. · Urgent hospital treatment is likely to be needed.

EYE
■ If this product comes in contact with the eyes: · Immediately hold eyelids apart and flush the eye continuously with running water. · Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.

SKIN
■ If skin or hair contact occurs: · Immediately flush body and clothes with large amounts of water, using safety shower if available. · Quickly remove all contaminated clothing, including footwear.

INHALED
· If fumes or combustion products are inhaled remove from contaminated area. · Lay patient down. Keep warm and rested.

NOTES TO PHYSICIAN
■ Treat symptomatically.
for poisons (where specific treatment regime is absent):
----------BASIC TREATMENT

· Establish a patent airway with suction where necessary.
· Watch for signs of respiratory insufficiency and assist ventilation as necessary.
Following acute or short term repeated exposure to hydrofluoric acid:
· Subcutaneous injections of Calcium Gluconate may be necessary around the burnt area. Continued application of Calcium Gluconate Gel or subcutaneous Calcium Gluconate should then continue for 3-4 days at a frequency of 4-6 times per day. If a "burning" sensation recurs, apply more frequently.
· Systemic effects of extensive hydrofluoric acid burns include renal damage, hypocalcemia and consequent cardiac arrhythmias. Monitor hematological, respiratory, renal, cardiac and electrolyte status at least daily. Tests should include FBE, blood gases, chest X-ray, creatinine and electrolytes, urine output, Ca ions, Mg ions and phosphate ions. Continuous ECG monitoring may be required.

Section 5 - FIRE FIGHTING MEASURES

Vapour Pressure (mmHG):	Not available
Upper Explosive Limit (%):	Not available
Specific Gravity (water=1):	1.69
Lower Explosive Limit (%):	Not available

EXTINGUISHING MEDIA
· Dry chemical powder.
· BCF (where regulations permit).
Do not use water.

FIRE FIGHTING
· Alert Emergency Responders and tell them location and nature of hazard.
· Wear full body protective clothing with breathing apparatus.
When any large container (including road and rail tankers) is involved in a fire, consider evacuation by 800 metres in all directions.

GENERAL FIRE HAZARDS/HAZARDOUS COMBUSTIBLE PRODUCTS

· Combustible.
· Slight fire hazard when exposed to heat or flame.
Combustion products include: carbon dioxide (CO_2), hydrogen fluoride, other pyrolysis products typical of burning organic material.
May emit poisonous fumes.

FIRE INCOMPATIBILITY

■ Avoid contamination with oxidizing agents i.e. nitrates, oxidizing acids,chlorine bleaches, pool chlorine etc. as ignition may result.

PERSONAL PROTECTION

Glasses:
Full face- shield.
Gloves:
Respirator:
Type BAX-P Filter of sufficient capacity

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS
· Remove all ignition sources.
· Clean up all spills immediately.
Any leak should be treated as a Major Spill
MAJOR SPILLS
· Clear area of personnel and move upwind.
· Alert Emergency Responders and tell them location and nature of hazard.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

· DO NOT allow clothing wet with material to stay in contact with skin.
· Avoid all personal contact, including inhalation.
· Wear protective clothing when risk of exposure occurs.

RECOMMENDED STORAGE METHODS

· Lined metal can, Lined metal pail/drum
· Plastic pail.
For low viscosity materials
· Drums and jerricans must be of the non-removable head type.
· Where a can is to be used as an inner package, the can must have a screwed enclosure.
· Material is corrosive to most metals, glass and other siliceous materials.

STORAGE REQUIREMENTS

· Store in an upright position.
· Store in original containers.
· Keep containers securely sealed.

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

Source	Material	TWA ppm	TWA mg/m³	STEL ppm	STEL mg/m³	Peak ppm	Peak mg/m³	TWA F/CC	Notes
Canada - Alberta Occupational Exposure Limits	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7						
Canada - British Columbia Occupational Exposure Limits	hexafluoroacetone (Hexafluoroacetone)	0.1							Skin; R
US NIOSH Recommended Exposure Limits (RELs)	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7						[skin]
Canada - Quebec Permissible Exposure Values for Airborne	hexafluoroacetone (Hexafluoroacetone)	0.1	0.68						

Contaminants (English)							
US ACGIH Threshold Limit Values (TLV)	hexafluoroacetone (Hexafluoroacetone)	0.1					TLV Basis: testicular & kidney damage
US - Vermont Permissible Exposure Limits Table Z-1-A Final Rule Limits for Air Contaminants	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7				
US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7				
US - Minnesota Permissible Exposure Limits (PELs)	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7				
US - California Permissible Exposure Limits for Chemical Contaminants	hexafluoroacetone (Hexafluoroacetone; 1,1,1,3,3,3-hexafluoro-2-propanone)	0.1	0.7				
US - Hawaii Air Contaminant Limits	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7	0.3	2		
US - Alaska Limits for Air Contaminants	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7				
Canada - Saskatchewan Occupational Health and Safety Regulations - Contamination Limits	hexafluoroacetone (Hexafluoroacetone)	0.1		0.3			Skin
Canada - Yukon Permissible Concentrations for Airborne Contaminant Substances	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7	0.3	2.1		
US - Washington Permissible exposure limits of air contaminants	hexafluoroacetone (Hexafluoroacetone)	0.1		0.3			
Canada - Nova Scotia Occupational Exposure Limits	hexafluoroacetone (Hexafluoroacetone)	0.1					TLV Basis: testicular & kidney damage
Canada - Prince Edward Island Occupational Exposure Limits	hexafluoroacetone (Hexafluoroacetone)	0.1					TLV Basis: testicular & kidney damage
Canada - Northwest Territories Occupational Exposure Limits (English)	hexafluoroacetone (Hexafluoroacetone)	0.1	0.68	0.3	2		

US - Michigan Exposure Limits for Air Contaminants	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7				
US - Oregon Permissible Exposure Limits (Z-1)	hexafluoroacetone (Hexafluoroacetone)	0.1	0.7				*
US - Minnesota Permissible Exposure Limits (PELs)	hydrogen fluoride (Hydrogen fluoride (as F))	3		6			
US ATSDR Minimal Risk Levels for Hazardous Substances (MRLs)	hydrogen fluoride (HYDROGEN FLUORIDE)	0.02					
Canada - British Columbia Occupational Exposure Limits	hydrogen fluoride (Hydrogen fluoride, as F)				2		
US ACGIH Threshold Limit Values (TLV)	hydrogen fluoride (Hydrogen fluoride)	0.5			2		Measured as F. TLV Basis: upper and lower respiratory tract, skin & eye irritation; fluorosis
US NIOSH Recommended Exposure Limits (RELs)	hydrogen fluoride (Hydrogen fluoride)	3	2.5		6	5	(Ceiling ([15-minute]))
Canada - Alberta Occupational Exposure Limits	hydrogen fluoride (Hydrogen fluoride, as F)	0.5	0.4		2	1.6	
US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants	hydrogen fluoride (Hydrogen fluoride (as F))	3		6			
US - Vermont Permissible Exposure Limits Table Z-1-A Transitional Limits for Air Contaminants	hydrogen fluoride (Hydrogen fluoride (as F))		See Table Z-2				
US - Vermont Permissible Exposure Limits Table Z-1-A Final Rule Limits for Air Contaminants	hydrogen fluoride (Hydrogen fluoride (as F))	3		6			
US - Idaho - Acceptable Maximum Peak Concentrations	hydrogen fluoride (Hydrogen Fluoride (Z37.26-1969))	3					
US - California Permissible Exposure Limits for Chemical Contaminants	hydrogen fluoride (Hydrogen fluoride, as F)	3	2.5	6			
US - Idaho - Limits for Air Contaminants	hydrogen fluoride (Hydrogen fluoride (as F))		[2]				

US - Alaska Limits for Air Contaminants	hydrogen fluoride (Hydrogen fluoride (as F))	3		6				
US - Michigan Exposure Limits for Air Contaminants	hydrogen fluoride (Hydrogen fluoride (as F))	3		6				
US - Hawaii Air Contaminant Limits	hydrogen fluoride (Hydrogen fluoride (as F))	3		6				
Canada - Yukon Permissible Concentrations for Airborne Contaminant Substances	hydrogen fluoride (Hydrogen fluoride)	3	2	3	2			
US - Washington Permissible exposure limits of air contaminants	hydrogen fluoride (Hydrogen fluoride)					3		
Canada - Saskatchewan Occupational Health and Safety Regulations - Contamination Limits	hydrogen fluoride (Hydrogen fluoride, (as F))	0.5						
Canada - Northwest Territories Occupational Exposure Limits (English)	hydrogen fluoride (Hydrogen fluoride (as F))	3	2.5	6	4.9			
US - Wyoming Toxic and Hazardous Substances Table Z-2 Acceptable ceiling concentration, Acceptable maximum peak above the acceptable ceiling concentration for an 8-hr shift	hydrogen fluoride (Hydrogen fluoride (Z37.28-1969))	3						
Canada - Quebec Permissible Exposure Values for Airborne Contaminants (English)	hydrogen fluoride (Hydrogen fluoride (as F))					3	2.6	
US - Oregon Permissible Exposure Limits (Z-2)	hydrogen fluoride (Hydrogen fluoride (Z37.28-1969))	3						
Canada - Nova Scotia Occupational Exposure Limits	hydrogen fluoride (Hydrogen fluoride)	0.5				2		Measured as F. TLV Basis: upper and lower respiratory tract, skin & eye irritation; fluorosis

Canada - Prince Edward Island Occupational Exposure Limits	hydrogen fluoride (Hydrogen fluoride)	0.5	2	Measured as F. TLV Basis: upper and lower respiratory tract, skin & eye irritation; fluorosis

ENDOELTABLE
The following materials had no OELs on our records

• hexafluoroacetone hydrate: CAS:13098-39-0 CAS:34202-69-2 CAS:10057-27-9 CAS:32836-39-8 CAS:677-71-4

PERSONAL PROTECTION




RESPIRATOR

Type BAX-P Filter of sufficient capacity
Consult your EHS staff for recommendations

EYE

· Chemical goggles.
· Full face shield.

HANDS/FEET

■ Wear chemical protective gloves, eg. PVC.
· When handling corrosive liquids, wear trousers or overalls outside of boots, to avoid spills entering boots.
Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include: such as:
· frequency and duration of contact,
· chemical resistance of glove material,
· glove thickness and
· dexterity
Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).
· When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.
· When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.
· Contaminated gloves should be replaced.
Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

OTHER

· Overalls.
· Eyewash unit.

ENGINEERING CONTROLS

■ Local exhaust ventilation usually required. If risk of overexposure exists, wear an approved respirator.
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Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL PROPERTIES

Liquid.
Mixes with water.
Acid.

State	Liquid	Molecular Weight	193.05
Melting Range (°F)	50- 59	Viscosity	Not Applicable
Boiling Range (°F)	Not available	Solubility in water (g/L)	Miscible
Flash Point (°F)	Not Available	pH (1% solution)	Not applicable
Decomposition Temp (°F)	Not Available	pH (as supplied)	Not applicable
Autoignition Temp (°F)	Not available	Vapour Pressure (mmHG)	Not available
Upper Explosive Limit (%)	Not available	Specific Gravity (water=1)	1.69
Lower Explosive Limit (%)	Not available	Relative Vapor Density (air=1)	1.65

Volatile Component (%vol)	100	Evaporation Rate	Fast

APPEARANCE

Hydrate form of the hligjhly toxic gas, hexafluoroacetone . Colourless, highly reactive, liquid or solid. Melts at 10 C. Non Flammable. HAZARD. The liquid has significant vapour pressure; i.e. readily volatile. Data is for sesquihydrate CAS RN: 13098-39-0 C3F6O.1.5H2O. Other forms of hydrate are; trihydrate CAS RN: 34202-69-2 C3F6O.3H2O monohydrate CAS RN: 677-71-4 C3F6O.H2O dihydrate CAS RN: 32836-39-8 C3F6O.2H2O and mixed hydrates CAS RN: 10057-27-9 C3F6O.xH2O The toxicity effects of hydrates closely follows hexafluoroacetone.

Section 10 - CHEMICAL STABILITY

CONDITIONS CONTRIBUTING TO INSTABILITY

· Presence of incompatible materials.
· Product is considered stable.

STORAGE INCOMPATIBILITY

· In presence of moisture, the material is corrosive to aluminium, zinc and tin producing highly flammable hydrogen gas.
· Avoid any contamination of this material as it is very reactive and any contamination is potentially hazardous.
Hydrogen fluoride:
· reacts violently with strong oxidisers, acetic anhydride, alkalis, 2-aminoethanol, arsenic trioxide (with generation of heat), bismuthic acid, calcium oxide, chlorosulfonic acid, cyanogen fluoride, ethylenediamine, ethyleneimine, fluorine (fluorine gas reacts vigorously with a 50% hydrofluoric acid solution and may burst into flame), nitrogen trifluoride, N-phenylazopiperidine, oleum, oxygen difluoride, phosphorus pentoxide, potassium permanganate, potassium tetrafluorosilicate(2-), beta-propiolactone, propylene oxide, sodium, sodium tetrafluorosilicate, sulfuric acid, vinyl acetate
· reacts (possibly violently) with aliphatic amines, alcohols, alkanolamines, alkylene oxides, aromatic amines, amides, ammonia, ammonium hydroxide, epichlorohydrin, isocyanates, metal acetylides, metal silicides, methanesulfonic acid, nitrogen compounds, organic anhydrides, oxides, silicon compounds, vinylidene fluoride
· attacks glass and siliceous materials, concrete, ceramics, metals (flammable hydrogen gas may be produced), metal alloys, some plastics, rubber coatings, leather, and most other materials with the exception of lead, platinum, polyethylene, wax.
Avoid reaction with oxidizing agents.

For incompatible materials - refer to Section 7 - Handling and Storage.

Section 11 - TOXICOLOGICAL INFORMATION

HEXAFLUOROACETONE HYDRATE

TOXICITY AND IRRITATION

■ unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.
■ Asthma-like symptoms may continue for months or even years after exposure to the material ceases. This may be due to a non-allergenic condition known as reactive airways dysfunction syndrome (RADS) which can occur following exposure to high levels of highly irritating compound. Key criteria for the diagnosis of RADS include the absence of preceding respiratory disease, in a non-atopic individual, with abrupt onset of persistent asthma-like symptoms within minutes to hours of a documented exposure to the irritant. A reversible airflow pattern, on spirometry, with the presence of moderate to severe bronchial hyperreactivity on methacholine challenge testing and the lack of minimal lymphocytic inflammation, without eosinophilia, have also been included in the criteria for diagnosis of RADS. RADS (or asthma) following an irritating inhalation is an infrequent disorder with rates related to the concentration of and duration of exposure to the irritating substance. Industrial bronchitis, on the other hand, is a disorder that occurs as result of exposure due to high concentrations of irritating substance (often particulate in nature) and is completely reversible after exposure ceases. The disorder is characterised by dyspnea, cough and mucus production.
HEXAFLUOROACETONE:
HEXAFLUOROACETONE HYDRATE:
■ Exposure to the material for prolonged periods may cause physical defects in the developing embryo (teratogenesis).
■ In subchronic inhalation studies, intermittent exposure to 6.9 mg/m3 hexafluoroacetone caused reversible kidney dysfunction and increased relative lung weight in rats and dogs, respectively. This concentration did not induce testicular effects in rats. In separate reproduction toxicity studies in which pregnant rats were exposed during organogenesis, minimal but statistically significant decreases in female offspring body weight were seen at exposure by inhalation to 0.76 mg/m3, and a higher incidence of hydronephrosis, one anophthalmic foetus and 2 stunted fetuses at a dermal dose of 0.75 mg /kg bw, the lowest concentration/dose tested.
Pregnant rats (n=24/group) were exposed to hexafluoroacetone concentrations of 0, 0.76, 6.9, or 48 mg/m3 (0.11, 1, 6.9 ppm), 6 hours/day, on gestational days 7 through 16. On gestational days 17 to 22, maternal weight gain in the high-concentration group was less than in the control group ($p<0.05$). This was attributed to embryolethality and an adverse effect on fetal weight in this group rather than to maternal toxicity. The mean number of live fetuses per litter was significantly decreased and the number and percentages of total and later resorptions were significantly increased in the high-concentration group. Late resorptions were also slightly, but significantly increased in the mid-concentration group. It is not clear whether the increase in late resorptions at the mid concentration is a compound-related effect. The weights of male, female, and combined fetuses were significantly lower than controls in both the mid- and high-concentration groups.
Malformations were significantly increased at the high concentration, and included increases in anasarca (subcutaneous oedema) and cleft soft palates. External developmental variations (oedema and subcutaneous haemorrhages) were also significantly increased in the high-concentration group. Skeletal variations consisting of extracervical and lumbar ribs were significantly increased at the mid and the high concentration. Variations due to retarded development, primarily delayed ossifications of the skull, vertebrae, ribs, and sternebrae were increased at the high concentration The maternal NOAEL was 0.76 mg/m3. A NOAEL for the conceptus could not be established. Based on a minimally decreased body weight in female foetuses, it was concluded that 0.76 mg/m3 (0.11 ppm) (the lowest concentration tested) is a lowest-observed-adverse-effect level (LOAEL) for developmental effects in rats.
Male rats were exposed to hexafluoroacetone concentrations of 0, 0.7, 6.9, or 83 mg/m3 (0, 0.1, 1, 12 ppm), 6 hours/day, 5 days/week, for 90

days (n=40/group).
After 30 days of exposure to 83 mg/m3 (12 ppm), rats showed lower body weight gain, testicular atrophy, and oligospermia or aspermia in the epididymal tubules. At 90 days of exposure, the testes showed severe atrophy with almost all seminiferous tubules affected. After a 28-day recovery period, regeneration of atrophic testes was evident but varied markedly among the exposed rats. At 84 days postexposure, spermatogenesis was still only partially restored. It can be concluded that inhalation exposure to 6.9 mg/m3 (1ppm) is an NOAEL for testicular effects in rats. In another study with the sesquihydrate, similar findings were reported. Histological evaluation of the testes revealed that spermatids followed by spermatocytes were the germ cells mostly affected; spermatogonia and Sertoli cells appeared to be less vulnerable. Possibly the altered lipid metabolism, in particular sterol metabolism, is associated with the development of hexafluoroacetone-induced testicular atrophy.
Hexafluoroacetone dihydrate was not mutagenic in the Ames assay, using S. typhimurium (no details presented) Hexafluoroacetone sesquihydrate was not mutagenic in the Ames assay, using S. typhimurium strains TA97, TA98, TA100 and TA1535, with and without rat- and hamster-liver metabolic activation.
HEXAFLUOROACETONE HYDRATE:

TOXICITY	IRRITATION
Oral (rat) LD50: 191 mg/kg	
Inhalation (rat) LC50: 275 ppm/3h	
Dermal (rat) TDLo: 55 mg/kg	
Oral (rat) LD50: 190 mg/kg	
Dermal (rabbit) LD50: 113 mg/kg	
as hexafluoroacetone Reproductive as trihydrate CAS RN: 34202-69-2 Somnolence, primary irritation, foetotoxicity, foetolethality, specific developmental abnormalities (central nervous system, eye, ear, craniofacial, musculoskeletal system, urogenital system) recorded.	

TOXICITY	IRRITATION
HEXAFLUOROACETONE:	
Oral (rat) LD50: 191 mg/kg	
Inhalation (rat) LC50: 275 ppm/3h	
Dermal (rat) TDLo: 55 mg/kg	
Oral (rat) LD50: 190 mg/kg	
Dermal (rabbit) LD50: 113 mg/kg	
as trihydrate CAS RN: 34202-69-2	
Somnolence, primary irritation, foetotoxicity, foetolethality, specific developmental abnormalities (central nervous system, eye, ear, craniofacial, musculoskeletal system, urogenital system) recorded.	
HYDROGEN FLUORIDE:	
Inhalation (human) LCLo: 50 ppm/30 m	Eye (human): 50 mg - SEVERE
Inhalation (man) TCLo: 100 mg/m³/1 m	
Inhalation (rat) LC50: 1276 ppm/1 h	

■ The material may produce severe irritation to the eye causing pronounced inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis.

SKIN

hexafluoroacetone	US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants - Skin	Skin Designation	X
hexafluoroacetone	US - Vermont Permissible Exposure Limits Table Z-1-A Final Rule Limits for Air Contaminants - Skin	Skin Designation	X
hexafluoroacetone	US - Washington Permissible exposure limits of air contaminants - Skin	Skin	X
hexafluoroacetone	US - Minnesota Permissible Exposure Limits (PELs) - Skin	Skin Designation	X
hexafluoroacetone	US - Hawaii Air Contaminant Limits - Skin Designation	Skin Designation	X
hexafluoroacetone	US OSHA Permissible Exposure Levels (PELs) - Skin	Skin Designation	X

hexafluoroacetone	Canada - Alberta Occupational Exposure Limits - Skin	Substance Interaction	1

Section 12 - ECOLOGICAL INFORMATION

This material and its container must be disposed of as hazardous waste.

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
hexafluoroacetone	HIGH		LOW	HIGH
hydrogen fluoride			LOW	

Section 13 - DISPOSAL CONSIDERATIONS

US EPA Waste Number & Descriptions

B. Component Waste Numbers
When hydrogen fluoride is present as a solid waste as a discarded commercial chemical product, off-specification species, as a container residue, or a spill residue, use EPA waste number U134 (waste code C,T).

Disposal Instructions

All waste must be handled in accordance with local, state and federal regulations.
¦ Puncture containers to prevent re-use and bury at an authorized landfill.
Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.
A Hierarchy of Controls seems to be common - the user should investigate:
· Reduction
· Reuse
· Recycling
· Disposal (if all else fails)
This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. If it has been contaminated, it may be possible to reclaim the product by filtration, distillation or some other means. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.
DO NOT allow wash water from cleaning equipment to enter drains. Collect all wash water for treatment before disposal.
· Recycle wherever possible or consult manufacturer for recycling options.
· Consult Waste Management Authority for disposal.

Section 14 - TRANSPORTATION INFORMATION

DOT:
Symbols: None Hazard class or Division: 6.1
Identification Numbers: UN2552 PG: II
Label Codes: 6.1 Special provisions: IB2, T7,
TP2
Packaging: Exceptions: 153 Packaging: Non- bulk: 202
Packaging: Exceptions: 153 Quantity limitations: 5 L
Passenger aircraft/rail:
Quantity Limitations: Cargo 60 L Vessel stowage: Location: B
aircraft only:
Vessel stowage: Other: 40
Hazardous materials descriptions and proper shipping names:
Hexafluoroacetone hydrate, liquid

Air Transport IATA:

ICAO/IATA Class: 6.1 ICAO/IATA Subrisk: None
UN/ID Number: 2552 Packing Group: II
Special provisions: None
Cargo Only
Packing Instructions: 611 Maximum Qty/Pack: 60 L
Passenger and Cargo Passenger and Cargo
Packing Instructions: 609 Maximum Qty/Pack: 5 L
Passenger and Cargo Limited Quantity Passenger and Cargo Limited Quantity
Packing Instructions: Y609 Maximum Qty/Pack: 1 L
Shipping Name: HEXAFLUOROACETONE HYDRATE, LIQUID

Maritime Transport IMDG:

IMDG Class: 6.1 IMDG Subrisk: None
UN Number: 2552 Packing Group: II
EMS Number: F-A , S-A Special provisions: None

Limited Quantities: 100 ml
Shipping Name: HEXAFLUOROACETONE HYDRATE, LIQUID

Section 15 - REGULATORY INFORMATION

hexafluoroacetone hydrate (CAS: 13098-39-0,34202-69-2,10057-27-9,32836-39-8,677-71-4) is found on the following regulatory lists;

"Canada Toxicological Index Service - Workplace Hazardous Materials Information System - WHMIS (English)"

Regulations for ingredients

hexafluoroacetone (CAS: 684-16-2,13098-39-0,34202-69-2,677-71-4,32836-39-8,10057-27-9) is found on the following regulatory lists;

"Canada - Alberta Occupational Exposure Limits","Canada - British Columbia Occupational Exposure Limits","Canada - Northwest Territories Occupational Exposure Limits (English)","Canada - Nova Scotia Occupational Exposure Limits","Canada - Prince Edward Island Occupational Exposure Limits","Canada - Quebec Permissible Exposure Values for Airborne Contaminants (English)","Canada - Saskatchewan Occupational Health and Safety Regulations - Contamination Limits","Canada - Yukon Permissible Concentrations for Airborne Contaminant Substances","Canada Ingredient Disclosure List (SOR/88-64)","Canada Non-Domestic Substances List (NDSL)","Canada Toxicological Index Service - Workplace Hazardous Materials Information System - WHMIS (English)","US - Alaska Limits for Air Contaminants","US - California Occupational Safety and Health Regulations (CAL/OSHA) - Hazardous Substances List","US - California Permissible Exposure Limits for Chemical Contaminants","US - California Proposition 65 - Reproductive Toxicity","US - Connecticut Hazardous Air Pollutants","US - Hawaii Air Contaminant Limits","US - Maine Chemicals of High Concern List","US - Massachusetts Oil & Hazardous Material List","US - Michigan Exposure Limits for Air Contaminants","US - Minnesota Hazardous Substance List","US - Minnesota Permissible Exposure Limits (PELs)","US - New Jersey Right to Know Hazardous Substances","US - Oregon Hazardous Materials","US - Oregon Permissible Exposure Limits (Z-1)","US - Pennsylvania - Hazardous Substance List","US - Rhode Island Hazardous Substance List","US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants","US - Vermont Permissible Exposure Limits Table Z-1-A Final Rule Limits for Air Contaminants","US - Vermont Permissible Exposure Limits Table Z-1-A Transitional Limits for Air Contaminants","US - Washington Permissible exposure limits of air contaminants","US - Wyoming List of Highly Hazardous Chemicals, Toxics and Reactives","US ACGIH Threshold Limit Values (TLV)","US Department of Homeland Security Chemical Facility Anti-Terrorism Standards - Chemicals of Interest","US DOE Temporary Emergency Exposure Limits (TEELs)","US EPA Acute Exposure Guideline Levels (AEGLs) - Interim","US NFPA 45 Fire Protection for Laboratories Using Chemicals - Flammability Characteristics of Common Compressed and Liquefied Gases","US NIOSH Recommended Exposure Limits (RELs)","US OSHA List of Highly Hazardous Chemicals, Toxics and Reactives","US Toxic Substances Control Act (TSCA) - Inventory","USA: Chemical Facility Anti-Terrorism Standards - List Appendix A - 6CFR 27"

hydrogen fluoride (CAS: 7664-39-3) is found on the following regulatory lists;

"Canada - Alberta Ambient Air Quality Objectives","Canada - Alberta Occupational Exposure Limits","Canada - British Columbia Occupational Exposure Limits","Canada - Northwest Territories Occupational Exposure Limits (English)","Canada - Nova Scotia Occupational Exposure Limits","Canada - Prince Edward Island Occupational Exposure Limits","Canada - Quebec Permissible Exposure Values for Airborne Contaminants (English)","Canada - Saskatchewan Occupational Health and Safety Regulations - Contamination Limits","Canada - Yukon Permissible Concentrations for Airborne Contaminant Substances","Canada Domestic Substances List (DSL)","Canada Environmental Quality Guidelines (EQGs) Air","Canada Ingredient Disclosure List (SOR/88-64)","Canada National Pollutant Release Inventory (NPRI)","Canada Toxicological Index Service - Workplace Hazardous Materials Information System - WHMIS (English)","OECD Representative List of High Production Volume (HPV) Chemicals","The Australia Group Export Control List: Chemical Weapons Precursors","US - Alaska Limits for Air Contaminants","US - California Air Toxics ""Hot Spots"" List (Assembly Bill 2588) Substances for which emissions must be quantified","US - California Occupational Safety and Health Regulations (CAL/OSHA) - Hazardous Substances List","US - California OEHHA/ARB - Acute Reference Exposure Levels and Target Organs (RELs)","US - California OEHHA/ARB - Chronic Reference Exposure Levels and Target Organs (CRELs)","US - California Permissible Exposure Limits for Chemical Contaminants","US - California Toxic Air Contaminant List Category II","US - Connecticut Hazardous Air Pollutants","US - Hawaii Air Contaminant Limits","US - Idaho - Acceptable Maximum Peak Concentrations","US - Idaho - Limits for Air Contaminants","US - Massachusetts Oil & Hazardous Material List","US - Michigan Exposure Limits for Air Contaminants","US - Minnesota Hazardous Substance List","US - Minnesota Permissible Exposure Limits (PELs)","US - New Jersey Right to Know Hazardous Substances","US - Oregon Hazardous Materials","US - Oregon Permissible Exposure Limits (Z-1)","US - Oregon Permissible Exposure Limits (Z-2)","US - Pennsylvania - Hazardous Substance List","US - Rhode Island Hazardous Substance List","US - Tennessee Occupational Exposure Limits - Limits For Air Contaminants","US - Vermont Hazardous Constituents","US - Vermont Hazardous wastes which are Discarded Commercial Chemical Products or Off-Specification Batches of Commercial Chemical Products or Spill Residues of Either","US - Vermont Permissible Exposure Limits Table Z-1-A Final Rule Limits for Air Contaminants","US - Vermont Permissible Exposure Limits Table Z-1-A Transitional Limits for Air Contaminants","US - Washington Dangerous waste constituents list","US - Washington Discarded Chemical Products List - ""U"" Chemical Products","US - Washington Permissible exposure limits of air contaminants","US - Wyoming List of Highly Hazardous Chemicals, Toxics and Reactives","US - Wyoming Toxic and Hazardous Substances Table Z1 Limits for Air Contaminants","US - Wyoming Toxic and Hazardous Substances Table Z-2 Acceptable ceiling concentration, Acceptable maximum peak above the acceptable ceiling concentration for an 8-hr shift","US ACGIH Threshold Limit Values (TLV)","US ATSDR Minimal Risk Levels for Hazardous Substances (MRLs)","US CERCLA Priority List of Hazardous Substances","US Clean Air Act - Hazardous Air Pollutants","US CWA (Clean Water Act) - List of Hazardous Substances","US CWA (Clean Water Act) - Reportable Quantities of Designated Hazardous Substances","US Department of Homeland Security Chemical Facility Anti-Terrorism Standards - Chemicals of Interest","US Department of Transportation (DOT) List of Hazardous Substances and Reportable Quantities - Hazardous Substances Other Than Radionuclides","US DOE Temporary Emergency Exposure Limits (TEELs)","US EPA Acute Exposure Guideline Levels (AEGLs) - Final","US EPA Master Testing List - Index I Chemicals Listed","US EPCRA Section 313 Chemical List","US FDA Indirect Food Additives: Adhesives and Components of Coatings - Substances for Use Only as Components of Adhesives - Adhesives","US List of Lists - Consolidated List of Chemicals Subject to EPCRA, CERCLA and Section 112(r) of the Clean Air Act","US NFPA 45 Fire Protection for Laboratories Using Chemicals - Flammability Characteristics

of Common Compressed and Liquefied Gases","US NIOSH Recommended Exposure Limits (RELs)","US OSHA List of Highly Hazardous Chemicals, Toxics and Reactives","US OSHA Permissible Exposure Levels (PELs) - Table Z1","US OSHA Permissible Exposure Levels (PELs) - Table Z2","US Postal Service (USPS) Hazardous Materials Table: Postal Service Mailability Guide","US RCRA (Resource Conservation & Recovery Act) - Hazardous Constituents - Appendix VIII to 40 CFR 261","US RCRA (Resource Conservation & Recovery Act) - List of Hazardous Wastes","US SARA Section 302 Extremely Hazardous Substances","US Toxic Substances Control Act (TSCA) - Inventory"

Section 16 - OTHER INFORMATION

LIMITED EVIDENCE

■ Cumulative effects may result following exposure*.
* (limited evidence).

ND

Substance CAS Suggested codes hexafluoroacetone 684- 16- 2

Ingredients with multiple CAS Nos

Ingredient Name CAS hexafluoroacetone hydrate 13098-39-0, 34202-69-2, 10057-27-9, 32836-39-8, 677-71-4 hexafluoroacetone 684-16-2, 13098-39-0, 34202-69-2, 677-71-4, 32836-39-8, 10057-27-9

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■ Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.
A list of reference resources used to assist the committee may be found at:
www.chemwatch.net/references.

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

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