

SAFETY DATA SHEET

Creation Date 02-Oct-2014 Revision Date 23-Feb-2022 Revision Number 6

1. Identification

Product Name 3,5-Bis(trifluoromethyl)phenylmagnesium bromide, 0.5M solution in

THF

Cat No.: AC392150000; AC392151000

Synonyms No information available

Recommended Use Laboratory chemicals.

Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410
Fair Lawn, NJ 07410

Tel: (201) 796-7100

Emergency Telephone Number For information US call: 001-800-ACROS-01 / Europe call: +32 14 57 52 11

Emergency Number **US:**001-201-796-7100 / **Europe:** +32 14 57 52 99 **CHEMTREC** Tel. No.**US:**001-800-424-9300 / **Europe:**001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids

Skin Corrosion/Irritation

Serious Eye Damage/Eye Irritation

Category 1

Category 2

Carcinogenicity

Category 2

Specific target organ toxicity (single exposure)

Category 3

Target Organs - Respiratory system, Central nervous system (CNS).

Label Elements

Signal Word

Danger

Hazard Statements

Highly flammable liquid and vapor

Causes severe skin burns and eye damage May cause respiratory irritation Causes serious eye irritation May cause drowsiness or dizziness Suspected of causing cancer



Precautionary Statements

Prevention

Obtain special instructions before use

Do not handle until all safety precautions have been read and understood

Use personal protective equipment as required

Do not breathe dust/fume/gas/mist/vapors/spray

Wash face, hands and any exposed skin thoroughly after handling

Wear eye/face protection

Use only outdoors or in a well-ventilated area

Keep away from heat/sparks/open flames/hot surfaces. - No smoking

Keep container tightly closed

Ground/bond container and receiving equipment

Use explosion-proof electrical/ventilating/lighting equipment

Use only non-sparking tools

Take precautionary measures against static discharge

Keep cool

Response

Immediately call a POISON CENTER or doctor/physician

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

Skin

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower

Wash contaminated clothing before reuse

Eyes

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

IF SWALLOWED: Rinse mouth. DO NOT induce vomiting

Fire

In case of fire: Use CO2, dry chemical, or foam for extinction

Storage

Store locked up

Store in a well-ventilated place. Keep container tightly closed

Disposa

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Reacts violently with water

May form explosive peroxides

WARNING. Cancer - https://www.p65warnings.ca.gov/.

3. Composition/Information on Ingredients

Component	CAS No	Weight %
Tetrahydrofuran	109-99-9	> 80

3,5-BIS(TRIFLUOROMETHYL)PHENYLMAGNESI	112981-69-8	< 20
UM BROMIDE		

4. First-aid measures

General Advice Show this safety data sheet to the doctor in attendance. Immediate medical attention is

required.

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes.

Immediate medical attention is required.

Skin Contact Wash off immediately with plenty of water for at least 15 minutes. Remove and wash

contaminated clothing and gloves, including the inside, before re-use. Call a physician

immediately.

Inhalation If not breathing, give artificial respiration. Remove from exposure, lie down. Do not use

mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory

medical device. Call a physician immediately.

Ingestion Do NOT induce vomiting. Clean mouth with water. Never give anything by mouth to an

unconscious person. Call a physician immediately.

Most important symptoms and

effects

Causes burns by all exposure routes. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Causes central nervous system

depression

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media CO₂, dry chemical, dry sand, alcohol-resistant foam. Water mist may be used to cool

closed containers.

Unsuitable Extinguishing Media DO NOT USE WATER

Flash Point -17 °C / 1.4 °F

Method - No information available

Autoignition Temperature

Explosion Limits

No information available

Upper No data available Lower No data available

Sensitivity to Mechanical Impact No information available Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors. The product causes burns of eyes, skin and mucous membranes. Reacts violently with water. Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

Hazardous Combustion Products

Carbon monoxide (CO₂). Hydrogen halides. Magnesium oxides. Gaseous hydrogen fluoride (HF). **Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

NFPA

Health **Flammability** Instability Physical hazards 2

Accidental release measures

Personal Precautions

Ensure adequate ventilation. Use personal protective equipment as required. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak. Remove all sources of ignition. Take precautionary measures against static discharges. Should not be released into the environment.

Environmental Precautions

Methods for Containment and Clean Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Do not expose spill to water. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

7. Handling and storage

Handling

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Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Do not allow contact with water. If peroxide formation is suspected, do not open or move container. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

Storage.

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat, sparks and flame. Keep away from water or moist air. Keep under nitrogen. Flammables area. Shelf life 12 months. May form explosive peroxides on prolonged storage. Containers should be dated when opened and tested periodically for the presence of peroxides. Should crystals form in a peroxidizable liquid, peroxidation may have occurred and the product should be considered extremely dangerous. In this instance, the container should only be opened remotely by professionals. Corrosives area. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH IDLH	Mexico OEL (TWA)
Tetrahydrofuran	TWA: 50 ppm	(Vacated) TWA: 200 ppm	IDLH: 2000 ppm	TWA: 200 ppm
	STEL: 100 ppm	(Vacated) TWA: 590 mg/m ³	TWA: 200 ppm	TWA: 590 mg/m ³
	Skin	(Vacated) STEL: 250 ppm	TWA: 590 mg/m ³	STEL: 250 ppm
		(Vacated) STEL: 735 mg/m ³	STEL: 250 ppm	STEL: 735 mg/m ³
		TWA: 200 ppm	STEL: 735 mg/m ³	_
		TWA: 590 mg/m ³	_	

Legend

ACGIH - American Conference of Governmental Industrial Hygienists OSHA - Occupational Safety and Health Administration NIOSH IDLH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures

Use only under a chemical fume hood. Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by

OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard

EN166.

Skin and body protectionWear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard

EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State Liquid
Appearance Dark brown

Odor No information available
Odor Threshold No information available
pH No information available

Melting Point/Range No data available

Boiling Point/Range 65 °C / 149 °F @ 760 mmHg

Flash Point -17 °C / 1.4 °F Evaporation Rate No information available

Flammability (solid,gas) Not applicable

Flammability or explosive limits

Upper
LowerNo data available
No data availableVapor PressureNo information availableVapor DensityNo information available

Specific Gravity 1.015

Solubility Reacts violently with water

Partition coefficient; n-octanol/water

No data available

Autoignition TemperatureNo information availableDecomposition TemperatureNo information availableViscosityNo information available

10. Stability and reactivity

Reactive Hazard Yes

Stability May form explosive peroxides. Moisture sensitive. Reacts violently with water.

Conditions to Avoid Keep away from open flames, hot surfaces and sources of ignition. Incompatible products.

Exposure to moist air or water. Exposure to moisture.

Incompatible Materials Strong oxidizing agents

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO2), Hydrogen halides, Magnesium oxides,

Gaseous hydrogen fluoride (HF)

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing. Reacts violently with water.

11. Toxicological information

Acute Toxicity

Product Information

Oral LD50 Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg. **Dermal LD50** Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg. Vapor LC50 Based on ATE data, the classification criteria are not met. ATE > 20 mg/l.

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Tetrahydrofuran	1650 mg/kg (Rat)	> 2000 mg/kg (Rabbit)	180 mg/L (Rat) 1 h
			53.9 mg/L (Rat) 4 h

Toxicologically Synergistic

No information available

Products

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation Causes burns by all exposure routes

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Limited evidence of a carcinogenic effect.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Tetrahydrofuran	109-99-9	Group 2B	Not listed	A3	X	A3
3,5-BIS(TRIFLUORO METHYL)PHENYLMA	112981-69-8	Not listed				
GNESIUM BROMIDE						

ACGIH: (American Conference of Governmental Industrial Hygienists)

A1 - Known Human Carcinogen

A2 - Suspected Human Carcinogen

A3 - Animal Carcinogen

ACGIH: (American Conference of Governmental Industrial Hygienists)

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system Central nervous system (CNS)

STOT - repeated exposure None known

Aspiration hazard No information available

delayed

Symptoms / effects,both acute and Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric layage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation: Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Causes central nervous system depression

Endocrine Disruptor Information

Component	EU - Endocrine Disrupters	EU - Endocrine Disruptors -	Japan - Endocrine Disruptor
	Candidate List	Evaluated Substances	Information
Tetrahydrofuran	Group III Chemical	Not applicable	Not applicable

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

This product contains the following substance(s) which are hazardous for the environment. Reacts with water so no ecotoxicity data for the substance is available.

		Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
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Г	Tetrahydrofuran	Not listed	2160 mg/l LC50 = 96 h	Not listed	EC50 48 h 3485 mg/l
	•		Pimephales promelas		EC50: >10000 mg/L/24h
			Leuciscus idus: LC50: 2820		
			mg/L/48h		

Persistence and Degradability

Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation

No information available.

Mobility

Will likely be mobile in the environment due to its volatility.

Component	log Pow
Tetrahydrofuran	0.45

13. Disposal considerations

Waste Disposal Methods

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

Component	RCRA - U Series Wastes	RCRA - P Series Wastes
Tetrahydrofuran - 109-99-9	U213	-

14. Transport information

DOT

UN-No UN2924

Proper Shipping Name Alcohols,n.o.s., (Ethanol, Methanol)

Technical Name Tetrahydrofuran, 3,5-BIS(TRIFLUOROMETHYL)PHENYLMAGNESIUM BROMIDE

Hazard Class 3 Subsidiary Hazard Class 8 Packing Group II

TDG

UN-No UN2924

Proper Shipping Name Flammable liquid, corrosive, n.o.s.

Hazard Class 3 Subsidiary Hazard Class 8 Packing Group II

<u>IATA</u>

UN-No UN2924

Proper Shipping Name Flammable liquid, corrosive, n.o.s.

Hazard Class 3
Subsidiary Hazard Class 8
Packing Group ||

IMDG/IMO

UN-No UN2924

Proper Shipping Name Flammable liquid, corrosive, n.o.s.

Hazard Class 3 Subsidiary Hazard Class 8 Packing Group II

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Tetrahydrofuran	109-99-9	X	ACTIVE	-
3,5-BIS(TRIFLUOROMETHYL)PH	112981-69-8	-	-	-
ENYLMAGNESIUM BROMIDE				

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed '-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)

Not applicable

TSCA 12(b) - Notices of Export

Component	CAS No	TSCA 12(b) - Notices of Export
Tetrahydrofuran	109-99-9	Section 4, 1 % de minimus concentration

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Tetrahydrofuran	109-99-9	Χ	-	203-726-8	Χ	Χ	Χ	Х	Χ	KE-33454
3,5-BIS(TRIFLUOROMETHYL)PH	112981-69-8	-	-	-	-	-		-	-	-
ENYLMAGNESIUM BROMIDE										

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

U.S. Federal Regulations

SARA 313 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and

Health Administration

Not applicable

CERCLA This material, as supplied, contains one or more substances regulated as a hazardous

substance under the Comprehensive Environmental Response Compensation and Liability

Act (CERCLA) (40 CFR 302)

Component	Hazardous Substances RQs	CERCLA EHS RQs
Tetrahydrofuran	1000 lb	-

California Proposition 65

This product contains the following Proposition 65 chemicals.

Co	Component CAS No		California Prop. 65	Prop 65 NSRL	Category	
Tetra	hydrofuran	109-99-9	Carcinogen	-	Carcinogen	

U.S. State Right-to-Know

Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
Tetrahydrofuran	X	X	X	-	X

U.S. Department of Transportation

Reportable Quantity (RQ): Y
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland

Security

This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH

Component	. ,	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	
Tetrahydrofuran	-	Use restricted. See item 75. (see link for restriction details)	-

https://echa.europa.eu/substances-restricted-under-reach

Safety, health and environmental regulations/legislation specific for the substance or mixture

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Tetrahydrofuran	109-99-9	Listed	Not applicable	Not applicable	Not applicable
3,5-BIS(TRIFLUOROMETHYL)PHENYLMAGNESIUM BROMIDE	112981-69-8	Not applicable	Not applicable	Not applicable	Not applicable

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Tetrahydrofuran	109-99-9	Not applicable	Not applicable	Not applicable	Not applicable
3,5-BIS(TRIFLUOROMETHYL)PHENYLMAGNESIUM BROMIDE	112981-69-8	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By Regulatory Affairs

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Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard

replacing the current legislation under 29 CFR 1910.1200 to align with the Globally

Harmonized System of Classification and Labeling of Chemicals (GHS).

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS