

MATERIAL SAFETY DATA SHEET

Date prepared: December 6, 2002

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1. Product and Company Identification

PRODUCT IDENTIFIERS: **Borane-tetrahydrofuran complex, 2M solution in tetrahydrofuran (BTHF2M)**

PRODUCT PART NUMBERS: 10001019 (bulk)

STABILIZER: 0.008M NaBH₄

PRODUCT USE: Hydroboration and reduction reactions

MANUFACTURED BY: Callery Chemical Company

Division of Mine Safety Appliances Company

PO Box 429; Pittsburgh, PA 15230

Callery Customer Service: 1-412-967-4141

Callery 24-Hour Telephone: 1-412-967-4100

Transportation Emergency: 1-800-424-9300 in USA or 1-703-527-3887 outside USA

2. Composition/Information on Ingredients

	<u>wt%</u>	<u>Synonym(s)</u>
Borane-tetrahydrofuran complex (CASRN: 14044-65-6)	~20	BTHF, THFB
Tetrahydrofuran (CASRN: 109-99-9)	~80	THF

OSHA REGULATORY STATUS: Hazardous by definition of Hazard Communication Standard, 29 CFR 1910.1200.

3. Hazards Identification

Indications of danger (Annex II): Highly flammable and Irritant

Nature of special risk attributed to dangerous substances (Annex III): R11, R14/15, R36/37/38, R19, R44

Safety advice concerning dangerous chemical substances (Annex IV): S2, S7/8, S16, S23, S29, S33, S43, S51

EMERGENCY OVERVIEW: Colorless liquid with tetrahydrofuran and diborane odor. Reacts violently with water, moist air, alcohols, acids, and other incompatible materials releasing flammable hydrogen gas which can ignite explosively. Extremely flammable liquid and vapor. Vapor may cause flash fire. Causes skin irritation. May cause eye and respiratory tract irritation and central nervous system depression with nausea, dizziness, and headache. May be absorbed through the skin. May cause liver and kidney effects. Evolves flammable and toxic diborane gas above 50°C. Tetrahydrofuran can form potentially explosive peroxides upon long standing in air.

Laboratory tests indicate that exposure to adiabatic conditions (i.e., conditions in which there is no heat transfer to or from a container's surroundings) at temperatures over 40°C may lead to a self-sustaining exothermic reaction that can cause a temperature increase. If the temperature under adiabatic conditions is allowed to reach approximately 60°C, a violent decomposition reaction may occur. This latter reaction can very rapidly evolve large quantities of heat, flammable hydrogen gas, and flammable and toxic diborane gas, resulting in fire, explosion, or dangerous pressures in sealed containers.

Handle as a hazard class 4.1, self-reactive hazardous material. The self-accelerating decomposition temperature (SADT) is estimated to be 40°C. See Section 10.

PHYSICAL HAZARDS: Reacts violently with water, moist air, alcohols, acids, and other incompatible materials releasing flammable hydrogen gas which can ignite explosively. Extremely flammable liquid and vapor. Vapor may cause flash fire. Evolves flammable and toxic diborane gas above 50°C. Tetrahydrofuran can form potentially explosive peroxides upon long standing in air.

POTENTIAL HEALTH EFFECTS: Causes skin irritation. May cause eye and respiratory tract irritation and central nervous system depression with nausea, dizziness, and headache. May be absorbed through the skin. May cause liver and kidney effects.

Primary Routes of Entry: Skin absorption, eye and skin contact, inhalation, ingestion

Target Organs: Eyes, skin, respiratory tract, central nervous system, kidneys, liver

Medical Conditions Generally Recognized as Aggravated by Exposure: Persons with preexisting skin, respiratory, liver and kidney conditions may be more susceptible to the effects of this product.

Carcinogenicity: Borane-tetrahydrofuran complex and tetrahydrofuran are not listed in the National Toxicology Program (NTP) Annual Report on Carcinogens, not found to be potential carcinogens in the International Agency for Research on Cancer (IARC) Monographs, and not listed as OSHA carcinogens.

POTENTIAL ENVIRONMENTAL EFFECTS: No environmental toxicity data for the product. See Section 12 for additional information.

4. First Aid Measures

SEND TO A PHYSICIAN IN ALL CASES.

Note: Immediately flushing with plenty of water is the appropriate eye and skin emergency first aid treatment for this water-reactive chemical. For the eye, it is extremely important that flushing with water (with the eyelids held open) begins within the first minute after borane-tetrahydrofuran complex has entered the eye and continues for the full 20 minutes. If large amounts of borane-tetrahydrofuran complex are involved, flammable fumes and solutions may be produced during the emergency first aid treatment procedure; therefore, emergency showers should be adequately ventilated and equipped to handle flammable fumes and solutions that emergency first aid treatment may generate.

Eyes: Immediately flush eyes with plenty of water for at least 20 minutes while holding eyelids open.

Skin: Immediately flush skin with plenty of water for at least 20 minutes while removing contaminated clothing and shoes. Dispose of contaminated clothing and shoes in compliance with all local, state, and federal laws and regulations.

Ingestion: For any accidental contamination of the mouth, gargle with water and rinse mouth thoroughly for at least 20 minutes. If swallowed, do not induce vomiting. Give demulcent such as milk, olive oil, or margarine in small amounts up to 2 or 3 ounces. Never give anything by mouth to an unconscious person.

Inhalation: Remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.

5. Fire Fighting Measures

FLAMMABLE PROPERTIES: Water reactive. Extremely flammable liquid and vapor. Closed containers exposed to fire conditions may present risk of overpressurization, rupture, explosion, or flammable and toxic diborane gas release. Handle as a hazard class 4.1, self-reactive hazardous material. The self-accelerating decomposition temperature (SADT) is estimated to be 40°C. See Section 10.

Flashpoint (closed cup): -26.9°C/-16.4°F for BTHF2M

Autoignition Temperature for BTHF2M: 75-78°C/167-172.4°F

EXTINGUISHING MEDIA: Use carbon dioxide or dry chemical.

DO NOT use water, foam, or halogenated extinguishing agents.

UNUSUAL FIRE AND EXPLOSION HAZARDS: Evolves flammable and toxic diborane gas above 50°C. Reacts violently with water, moist air, alcohols, acids and other incompatible materials liberating flammable hydrogen gas which can ignite explosively. See Section 10. See also STABILITY TO AIR in Section 9. THF vapor is heavier than air and may travel along the ground to a distant source of ignition and flashback. If THF is distilled from the reaction mixture, potentially explosive peroxides may form in the distillate. Distillate must be inhibited or protected from air.

PROTECTION OF FIRE FIGHTERS: Wear full protective clothing, including protective gloves and boots. For respiratory protection, wear a NIOSH approved self-contained breathing apparatus with full facepiece operated in a positive-pressure mode.

6. Accidental Release Measures

PROCEDURES FOR CLEANUP: Wear recommended personal protective equipment. Be prepared to fight fire. Eliminate ignition sources. Do not flush spill to drain. Mix with large amounts of DRY soda ash. Using non-sparking tools, scoop solids into a DRY metal container, properly label, and cover. Take immediately to a waste handling area. If contaminated, flammable hydrogen gas can evolve and cause fire, explosion, or pressure buildup in container. Properly dispose of all residues immediately. Handle in compliance with all local, state, and federal laws and regulations. The reportable quantity for tetrahydrofuran is 1000 pounds.

7. Handling And Storage

HYGIENIC PRACTICES: Avoid breathing vapor or mist. Use only with adequate ventilation. Keep container tightly closed. Avoid contact with eyes, skin, and clothing. Wash thoroughly after handling.

STORAGE: To prevent product decomposition and avoid circumstances discussed in Section 10, refrigerate at 5°C or lower. Handle and store in a DRY closed system under DRY nitrogen gas. Do not store residues. Properly dispose of all residues immediately.

WORK PRACTICES: See Section 10 for additional information on conditions to avoid. Keep away heat, sparks, flame and any possible contact with water, moist air, alcohols, acids, and other incompatible materials. Do not expose to air. Handle and store in a closed system under DRY nitrogen gas. Use DRY nitrogen gas to inert containers, transfer lines, vessels, tanks, etc., such that the atmosphere stays below 3% oxygen. Use non-sparking tools when opening or closing containers. Bond and ground all systems when handling. Since empty containers retain product residue, follow label warnings even after container is emptied.

PROTECTIVE MEASURES DURING REPAIR AND MAINTENANCE OF CONTAMINATED EQUIPMENT: See Section 8.

8. Exposure Controls/Personal Protection

ENGINEERING CONTROLS: See Section 10 for additional information on conditions to avoid. Maintain a leakproof system. Use packless valves, welded piping, and other leakproof construction. Handle in a closed system under DRY nitrogen gas. Provide adequate local exhaust ventilation to maintain worker exposure below exposure limits. Prevent electrostatic charge buildup by using common bonding and grounding techniques. Use DRY nitrogen gas to inert containers, transfer lines, vessels, tanks, etc., such that the atmosphere stays below 3% oxygen.

EXPOSURE CONTROLS: None established for the mixture.

For tetrahydrofuran: ACGIH TLV-TWA: 200 ppm

ACGIH TLV-STEL: 250 ppm

OSHA PEL-TWA: 200 ppm (590 mg/m³)

ACGIH has proposed a Biological Exposure Index (TLV-BEI) for tetrahydrofuran.

The IDLH for tetrahydrofuran is 2000 ppm.

Odor thresholds of 2 ppm and 7.4 ppm have been reported for tetrahydrofuran.

For diborane:

OSHA PEL-TWA: 0.1 ppm (0.1 mg/m³)

ACGIH TLV-TWA: 0.1 ppm

The IDLH for diborane is 15 ppm.

Odor threshold of 2.5 ppm has been reported for diborane.

PERSONAL PROTECTIVE EQUIPMENT:

Normal Use & Handling: When exposure to eyes and skin is possible, wear chemical protective goggles with a faceshield and flame-retardant protective clothing. Glove permeation data does not exist for this mixture. Exposure limits have not been established for Borane-tetrahydrofuran complex in tetrahydrofuran. When inhalation of vapor or mist is possible, wear a NIOSH-approved self-contained breathing apparatus with full facepiece operated in a positive-pressure mode. Eye wash and safety showers must be available and in good working order.

Emergency Handling: For firefighting, wear full protective clothing, including protective gloves and boots. For chemical spills, wear special protective clothing (vapor-protective suit with additional chemical flash fire escape protection, as specified in NFPA 991). For respiratory protection, wear a NIOSH-approved self-contained breathing apparatus with full facepiece operated in a positive-pressure mode.

9. Physical And Chemical Properties

APPEARANCE: Colorless liquid

ODOR: Tetrahydrofuran and diborane odor

BOILING POINT: Evolves flammable and toxic diborane gas before boiling (at temperatures as low as 112°F/50°C)

THF boils at 151°F/66°C at 760 mm Hg.

VAPOR DENSITY: 2.5 for THF

DENSITY: 0.875g/ml @ 25°C for BTHF2M

STABILITY TO AIR: Reacts with oxygen and moisture in air.

FORMULA WEIGHT: 85.94 g/mol

FORMULA: (CH₂)₄O:BH₃ in (CH₂)₄O

10. Stability And Reactivity

STABILITY (CONDITIONS TO AVOID): Keep away from heat, sparks, and flame. Per Section 7, refrigerate at 5°C or lower.

Laboratory tests (isothermal adiabatic Dewar and accelerating rate calorimetry tests) indicate that exposure to adiabatic conditions at temperatures over 40°C may lead to a self-sustaining exothermic reaction that can cause a temperature increase. If the temperature under adiabatic conditions is allowed to reach approximately 60°C, a violent decomposition reaction may occur (as indicated by further adiabatic laboratory tests (isothermal and dynamic accelerating rate calorimetry, and adiabatic isothermal Dewar tests)). This latter reaction can very rapidly evolve large quantities of heat, flammable hydrogen gas, and flammable and toxic diborane gas, resulting in fire, explosion, or dangerous pressures in sealed containers.

Laboratory data indicate that the material is capable of self-accelerating decomposition from 40°C under adiabatic conditions. Therefore, handle as a hazard class 4.1, self-reactive hazardous material with a self-accelerating decomposition temperature (SADT) of 40°C.

BTHF2M is not impact sensitive according to the criteria outlined in UN Test 3(a)(v), Section 13, UN Manual of Test and Criteria (3rd Revised Edition). However, testing at approximately 10 times the height prescribed by this test resulted in a decomposition reaction, including ignition, presumably due to an adiabatic temperature rise from compression.

INCOMPATIBILITY (SPECIFIC MATERIALS TO AVOID): Avoid unintended reactions with any chemical including, but not limited to, water, moist air, alcohols, acids, acid chlorides, acid anhydrides, oxygen, oxidizers, and some precious metal catalysts.

HAZARDOUS DECOMPOSITION PRODUCTS: Hydrogen, diborane, carbon monoxide, carbon dioxide, boron oxides, boranes.

HAZARDOUS POLYMERIZATION: Not expected to occur.

11. Toxicological Information

This product is a mixture which has not been tested for health hazards. The assumption is made in the OSHA Hazard Communication Standard that an untested mixture will present the same health hazards as do the components which comprise one percent or more. Health hazard information for all components is therefore included as part of this MSDS.

Borane-tetrahydrofuran complex has been shown to be an in vitro mutagen. No other information found for borane-tetrahydrofuran complex.

Tetrahydrofuran (THF) is a strong eye and respiratory irritant. Inhalation of vapors can cause central nervous system effects such as nausea, headache, dizziness, drowsiness, narcosis, and loss of feeling. THF may cause liver and kidney effects. THF may be absorbed through the skin.

Diborane is a gas that is toxic by inhalation, may cause eye irritation, and may cause central nervous system effects. Diborane gas acts primarily as an irritant to the respiratory system. Symptoms of acute exposure are respiratory distress, chest tightness, difficulty in breathing, non-productive coughing and wheezing, and sometimes nausea. Symptoms appear within a few minutes. In cases of mild exposure, they may last less than an hour; in more severe exposures, generally three to five days. Secondary infections were reported in some persons needing treatment. Chronic respiratory distress was present in two persons from recurring diborane exposure; it was believed to be due to a hypersensitivity reaction.

Exposure to low concentrations of diborane over a prolonged time period can cause lightheadedness, headache, fatigue, drowsiness, tremors, vertigo, chills, and sometimes fever; a cough and chest tightness may be present. Symptoms lasted from five days to three weeks.

The odor of diborane is unique and offers some warning, but potentially hazardous concentrations which cannot be detected by smell can exist in air. The odor detection threshold is 3.2 ppm or 3.7 mg/m³. In addition, prolonged exposure to diborane can temporarily impair the sense of smell.

TOXICITY DATA: No information found for the product.

12. Ecological Information

ECOLOGICAL DATA: No environmental toxicity data for the product.

If released to the atmosphere, tetrahydrofuran will exist solely in the vapor phase in the ambient atmosphere based on a measured vapor pressure of 162 mm Hg at 25°C. Vapor-phase tetrahydrofuran is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals and nitrate radicals with half-lives of about 1 and 3 days, respectively. Measured Koc values of 23 and 18 indicate that tetrahydrofuran will have very high mobility in soil. Volatilization from moist and dry soil surfaces may occur based on a measured Henry's Law constant of 7.05X10⁻⁵ atm-cu m/mole and tetrahydrofuran's measured vapor pressure, respectively. Tetrahydrofuran is expected to biodegrade under aerobic conditions but may be resistant to biodegradation in anaerobic environments. In the modified MITI screening test, tetrahydrofuran at 30 mg/l was completely biodegraded in 14 days using an activated sludge inoculum. The EEC

manometric respirometric method, tested in 22 different laboratories, gave a mean of 34% of the theoretical BOD within 28 days. Tetrahydrofuran at 50 mg C/l was resistant to anaerobic biodegradation with a lag period of greater than 60 days using a primary digesting sludge as an inoculum; no gas production was seen during this time. Tetrahydrofuran is not expected to adsorb to suspended matter in the water based on its measured Koc values. Tetrahydrofuran should volatilize from water surfaces given its Henry's Law constant. Estimated half-lives for a model river and model lake are 13 hours and 6 days, respectively. An estimated BCF value of 1 suggests that tetrahydrofuran will not bioconcentrate in aquatic organisms.

13. Disposal Considerations

WASTE DISPOSAL: Do not flush to sewer. Dispose in compliance with all local, state, and federal laws and regulations.

14. Transport Information

DO NOT ship. Contact Callery Chemical Company at 1-412-967-4141

15. Regulatory Information

TSCA: Borane-tetrahydrofuran complex and tetrahydrofuran are listed on the TSCA Public Inventory.

SARA 313 INFORMATION: Borane-tetrahydrofuran complex does not contain a toxic chemical or chemicals subject to the reporting requirements of section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 and 40 CFR 372.

CERCLA/SUPERFUND: The reportable quantity (RQ) for tetrahydrofuran is 1000 pounds.

EINECS: 237-881-8 for borane-tetrahydrofuran complex, 203-726-8 for tetrahydrofuran

EUROPEAN LABEL INFORMATION:

Symbols: F, Xi

Indications of danger (Annex II): Highly flammable, irritant

Nature of special risk attributed to dangerous substances (Annex III):

R11	Highly flammable.
R14/15	Reacts violently with water, liberating highly flammable gases.
R36/37/38	Irritating to eyes, respiratory system, and skin.
R19	May form explosive peroxides.
R44	Risk of explosion if heated under confinement.

Safety advice concerning dangerous chemical substances (Annex IV):

S2	Keep out of reach of children.
S7/8	Keep container tightly closed and dry.
S16	Keep away from sources of ignition.
S23	Do not breathe gas/fumes/vapour/spray.
S29	Do not empty into drains.
S33	Take precautionary measures against static discharges.
S43	In case of fire, use dry chemical or carbon dioxide. Never use water.
S51	Use only in well-ventilated areas.

CANADA: This mixture contains tetrahydrofuran, a chemical listed on the WHMIS Ingredient Disclosure List.

CALIFORNIA: This product does not contain a chemical known to the State of California to cause cancer.

NEW JERSEY: This mixture contains tetrahydrofuran, a chemical listed on the New Jersey Department of Health Hazard Right-to-Know Program Hazardous Substance List as a special health hazard.

PENNSYLVANIA: This mixture contains tetrahydrofuran and is subject to the Pennsylvania Worker and Community Right-to-Know Act.

16. Other Information

MSDS STATUS: Revised Sections 1, 2, 3, 5, 7, 8, 9, 10, 11, 14, 15, and 16.

WARNING: This is a dangerous chemical product. By following the directions and warnings provided with this product, the dangers associated with the use of this product can be greatly reduced but never entirely eliminated. Callery Chemical Company makes no warranties, expressed or implied, with respect to this product and EXPRESSLY DISCLAIMS THE WARRANTY OF MERCHANTABILITY AND ANY WARRANTY OF FITNESS FOR A PARTICULAR PURPOSE. Users assume all risks in handling, using or storing this product.

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