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

1.1 Product identifiers

Product name: Hexadecyltrimethylammonium bromide

Product Number: H5882
Brand: Sigma
CAS-No.: 57-09-0

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

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

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

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

Acute toxicity, Oral (Category 4), H302
Skin irritation (Category 2), H315
Serious eye damage (Category 1), H318
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335
Specific target organ toxicity - repeated exposure, Oral (Category 2), Gastrointestinal tract, H373
Short-term (acute) aquatic hazard (Category 1), H400
Long-term (chronic) aquatic hazard (Category 1), H410

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Sigma - H5882
2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms: Cetrimonium bromide
            Palmityltrimethylammonium bromide
            CTAB
            Cetyltrimethylammonium bromide

Formula: C19H42N.Br
Molecular weight: 364.45 g/mol
CAS-No.: 57-09-0
EC-No.: 200-311-3
### SECTION 4: First aid measures

#### 4.1 Description of first-aid measures

**General advice**
Show this material safety data sheet to the doctor in attendance.

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

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

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

**If swallowed**
After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media

**Suitable extinguishing media**
Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.
5.2 **Special hazards arising from the substance or mixture**
Carbon oxides
Nitrogen oxides (NOx)
Hydrogen bromide gas
Combustible.
Vapors are heavier than air and may spread along floors.
Forms explosive mixtures with air on intense heating.
Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 **Advice for firefighters**
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **Further information**
Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 **Environmental precautions**
Do not let product enter drains.

6.3 **Methods and materials for containment and cleaning up**
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

6.4 **Reference to other sections**
For disposal see section 13.

SECTION 7: Handling and storage

7.1 **Precautions for safe handling**
For precautions see section 2.2.

7.2 **Conditions for safe storage, including any incompatibilities**
**Storage conditions**
Tightly closed. Dry.

**Storage class**
Storage class (TRGS 510): 11: Combustible Solids

7.3 **Specific end use(s)**
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.
SECTION 8: Exposure controls/personal protection

8.1 Control parameters

*Ingredients with workplace control parameters*
Contains no substances with occupational exposure limit values.

8.2 Exposure controls

*Appropriate engineering controls*
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

**Personal protective equipment**

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

**Skin protection**
This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

- **Full contact**
  - Material: Nitrile rubber
  - Minimum layer thickness: 0.11 mm
  - Break through time: 480 min
  - Material tested: KCL 741 Dermatril® L

- **Splash contact**
  - Material: Nitrile rubber
  - Minimum layer thickness: 0.11 mm
  - Break through time: 480 min
  - Material tested: KCL 741 Dermatril® L

**Body Protection**
protective clothing

**Respiratory protection**
Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**
Do not let product enter drains.
SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: solid
   Color: white

b) Odor
   weak

c) Odor Threshold
   No data available

d) pH
   5.0 - 7 at 36.4 g/l at 25 °C (77 °F)

e) Melting point/freezing point
   Melting point/range: 248 - 251 °C (478 - 484 °F)

f) Initial boiling point and boiling range
   No data available

g) Flash point
   244 °C (471 °F) - closed cup

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   No data available

k) Vapor pressure
   No data available

l) Vapor density
   No data available

m) Density
   2.30 g/cm3
   Relative density
   No data available

n) Water solubility
   36.4 g/l at 20 °C (68 °F) - completely soluble

o) Partition coefficient: n-octanol/water
   log Pow: 2.26 - (Lit.), Bioaccumulation is not expected.

p) Autoignition temperature
   210 °C (410 °F) at 0.3 hPa

q) Decomposition temperature
   No data available

r) Viscosity
   No data available

s) Explosive properties
   No data available

t) Oxidizing properties
   none

9.2 Other safety information

Surface tension
   39 mN/m at 25 °C (77 °F)
SECTION 10: Stability and reactivity

10.1 Reactivity
Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.
The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

10.2 Chemical stability
The product is chemically stable under standard ambient conditions (room temperature).

10.3 Possibility of hazardous reactions
Violent reactions possible with:
Strong oxidizing agents
Caution! In contact with nitrites, nitrates, nitrous acid possible liberation of nitrosamines!

10.4 Conditions to avoid
Strong heating.

10.5 Incompatible materials
No data available

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - female - 1,550 mg/kg
(OECD Test Guideline 401)
Remarks: (in analogy to similar products)
The value is given in analogy to the following substances: Hexadecyltrimethylammonium chloride
Inhalation: No data available
Inhalation: Irritating to respiratory system.
LD50 Dermal - Rabbit - male and female - 2,150 mg/kg
Remarks: (in analogy to similar products)
(ECHA)
The value is given in analogy to the following substances: Hexadecyltrimethylammonium chloride
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Irritating to skin. - 24 h
Remarks: (ECHA)

Serious eye damage/eye irritation
Eyes - Rabbit
Result: Causes serious eye damage.
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

### 11.2 Additional Information

**Repeated dose toxicity - Rabbit** - male and female - Dermal - 28 d - LOAEL (Lowest observed adverse effect level) - 10 mg/kg
Remarks: (in analogy to similar products)

Repeated dose toxicity - Rat - male and female - Oral - 28 d - NOAEL (No observed adverse effect level) - 100 mg/kg
Remarks: (as aqueous solution)
(ECHA)

RTECS: BQ7875000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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**SECTION 12: Ecological information**

#### 12.1 Toxicity

**Toxicity to fish**
semi-static test LC50 - Danio rerio (zebra fish) - 0.2 mg/l - 96 h
(OECD Test Guideline 203)

Sigma - H5882
Toxicity to daphnia and other aquatic invertebrates semi-static test EC50 - Daphnia magna (Water flea) - 0.037 mg/l - 48 h (OECD Test Guideline 202)

Toxicity to algae static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 0.00411 mg/l - 72 h (OECD Test Guideline 201)

static test NOEC - Desmodesmus subspicatus (green algae) - 0.001 mg/l - 72 h (OECD Test Guideline 201)

Toxicity to bacteria EC50 - activated sludge - 19 mg/l Remarks: (ECHA)

Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity) NOEC - Daphnia magna (Water flea) - 0.023 mg/l - 21 d (OECD Test Guideline 211)

12.2 Persistence and degradability
Biodegradability aerobic Chemical oxygen demand - Exposure time 11 d Result: 100 % - Readily biodegradable. (OECD Test Guideline 301E)

12.3 Bioaccumulative potential
Bioaccumulation Cyprinus carpio (Carp) - 8 Weeks - 0.05 mg/l(N-Cetyl-N’N’N-trimethylammonium bromide)

Bioconcentration factor (BCF): 407 - 741
Due to the distribution coefficient n-octanol/water, accumulation in organisms is not expected.

12.4 Mobility in soil
No data available

12.5 Results of PBT and vPvB assessment
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties
No data available

12.7 Other adverse effects
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Very toxic to aquatic life.
SECTION 13: Disposal considerations

13.1 Waste treatment methods

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

SECTION 14: Transport information

DOT (US)
Not dangerous goods

IMDG
UN number: 3077  Class: 9  Packing group: III  EMS-No: F-A, S-F
Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (N-Cetyl-N'N'N-trimethylammonium bromide)
Marine pollutant: yes
Marine pollutant: no

IATA
UN number: 3077  Class: 9  Packing group: III
Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (N-Cetyl-N'N'N-trimethylammonium bromide)

Further information
EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids. Packages smaller than or equal to 5 kg / L, not dangerous goods of Class 9

SECTION 15: Regulatory information

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

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.
SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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