# Thermo Fisher SCIENTIFIC

# SAFETY DATA SHEET

Creation Date 02-Oct-2009 Revision Date 28-Jul-2022 Revision Number 3

# SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

## 1.1. Product identifier

Product Description: (1-Hexadecyl)trimethylammonium bromide

Cat No. : A15235

Synonyms Cetyltrimethylammonium bromide; Cetrimonium bromide; CTABr

 CAS No
 57-09-0

 EC No
 200-311-3

 Molecular Formula
 C19 H42 Br N

REACH registration number -

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

Recommended Use Laboratory chemicals.
Uses advised against No Information available

## 1.3. Details of the supplier of the safety data sheet

Company Alfa Aesar

Avocado Research Chemicals, Ltd.

Shore Road

Port of Heysham Industrial Park Heysham, Lancashire LA3 2XY

United Kingdom

Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608

E-mail address uktech@alfa.com

www.alfa.com

Product Safety Department

1.4. Emergency telephone number

Call Carechem 24 at

+44 (0) 1865 407333 (English only); +44 (0) 1235 239670 (Multi-language)

# **SECTION 2: HAZARDS IDENTIFICATION**

## 2.1. Classification of the substance or mixture

## CLP Classification - Regulation (EC) No 1272/2008

# **Physical hazards**

Based on available data, the classification criteria are not met

#### (1-Hexadecyl)trimethylammonium bromide

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#### **Health hazards**

Acute oral toxicity
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Specific target organ toxicity - (single exposure)
Specific target organ toxicity - (repeated exposure)
Specific target organ toxicity - (repeated exposure)
Category 2 (H373)

#### **Environmental hazards**

Acute aquatic toxicity
Chronic aquatic toxicity
Category 1 (H400)
Category 1 (H410)

Full text of Hazard Statements: see section 16

#### 2.2. Label elements



Signal Word

**Danger** 

#### **Hazard Statements**

H302 - Harmful if swallowed

H315 - Causes skin irritation

H318 - Causes serious eye damage

H335 - May cause respiratory irritation

H373 - May cause damage to organs through prolonged or repeated exposure

H410 - Very toxic to aquatic life with long lasting effects

## **Precautionary Statements**

P301 + P330 + P331 - IF SWALLOWED: rinse mouth. Do NOT induce vomiting

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P310 - Immediately call a POISON CENTER or doctor/physician

P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing

P280 - Wear protective gloves/protective clothing/eye protection/face protection

## 2.3. Other hazards

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB) No information available

Toxic to terrestrial vertebrates

# **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

## 3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - Regulation (EC) No
			3	1272/2008

## (1-Hexadecyl)trimethylammonium bromide

Hexadecyltrimethylammonium bromide	57-09-0	EEC No. 200-311-3	<=100	Acute Tox. 4 (H302) Skin Irrit. 2 (H315) Eye Dam. 1 (H318) STOT SE 3 (H335) STOT RE 2 (H373) Aquatic Acute 1 (H400)
				Aquatic Chronic 1 (H410)

Component	Specific concentration limits (SCL's)	M-Factor	Component notes
Hexadecyltrimethylammonium bromide	Skin Irrit. 2 : C ≥ 2.5 %	10	-

REACH registration number -
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Full text of Hazard Statements: see section 16

# **SECTION 4: FIRST AID MEASURES**

#### 4.1. Description of first aid measures

General Advice If symptoms persist, call a physician.

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

medical attention.

**Skin Contact** Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists,

call a physician.

**Ingestion** Clean mouth with water and drink afterwards plenty of water. Get medical attention if

symptoms occur.

**Inhalation** Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if

symptoms occur.

Self-Protection of the First Aider Ensure that medical personnel are aware of the material(s) involved, take precautions to

protect themselves and prevent spread of contamination.

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

None reasonably foreseeable. Causes severe eye damage.

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

Notes to Physician Treat symptomatically.

# **SECTION 5: FIREFIGHTING MEASURES**

## 5.1. Extinguishing media

# Suitable Extinguishing Media

Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam.

# Extinguishing media which must not be used for safety reasons

No information available.

# 5.2. Special hazards arising from the substance or mixture

#### (1-Hexadecyl)trimethylammonium bromide

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Thermal decomposition can lead to release of irritating gases and vapors. Do not allow run-off from fire-fighting to enter drains or water courses.

#### **Hazardous Combustion Products**

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO2), Hydrogen halides.

## 5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

## **SECTION 6: ACCIDENTAL RELEASE MEASURES**

#### 6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

#### 6.2. Environmental precautions

Do not flush into surface water or sanitary sewer system. Do not allow material to contaminate ground water system. Prevent product from entering drains. Local authorities should be advised if significant spillages cannot be contained.

#### 6.3. Methods and material for containment and cleaning up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

#### 6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

# **SECTION 7: HANDLING AND STORAGE**

#### 7.1. Precautions for safe handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid dust formation. Avoid ingestion and inhalation.

## **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

## 7.2. Conditions for safe storage, including any incompatibilities

Keep containers tightly closed in a dry, cool and well-ventilated place. Protect from moisture. Store under an inert atmosphere.

Technical Rules for Hazardous Substances (TRGS) 510 Class 11 Storage Class (LGK) (Germany)

## 7.3. Specific end use(s)

Use in laboratories

# **SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION**

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## 8.1. Control parameters

## **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

## **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

## Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

See table for values

Component	Acute effects local (Dermal)	Acute effects systemic (Dermal)	Chronic effects local (Dermal)	Chronic effects systemic (Dermal)
Hexadecyltrimethylammonium				DNEL = 0.4mg/kg
bromide				bw/day
57-09-0 ( <=100 )				_

Component	Acute effects local (Inhalation)	Acute effects systemic (Inhalation)	Chronic effects local (Inhalation)	Chronic effects systemic (Inhalation)
Hexadecyltrimethylammonium bromide	$DNEL = 0.05 mg/m^3$			
57-09-0 ( <=100 )				

# **Predicted No Effect Concentration (PNEC)**

See values below.

Component	Fresh water	Fresh water	Water Intermittent	Microorganisms in	Soil (Agriculture)
		sediment		sewage treatment	
Hexadecyltrimethylammoni	$PNEC = 0.022 \mu g/L$		PNEC = $0.4\mu g/L$	PNEC = 0.19mg/L	PNEC = 0.21 mg/kg
um bromide					soil dw
57-09-0 ( <=100 )					

Component	Marine water	Marine water sediment	Marine water intermittent	Food chain	Air
Hexadecyltrimethylammoni	$PNEC = 0.0022 \mu g/L$				
um bromide					
57-09-0 ( <=100 )					

# 8.2. Exposure controls

#### **Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

**Eye Protection** Goggles (European standard - EN 166)

Hand Protection Protective gloves

#### (1-Hexadecyl)trimethylammonium bromide

Glove material Breakthrough time Glove thickness EU standard Glove comments

Nitrile rubber See manufacturers - EN 374 (minimum requirement)

Neoprene recommendations

Natural rubber

PVC

Skin and body protection

Wear appropriate protective gloves and clothing to prevent skin exposure.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

**Respiratory Protection** No protective equipment is needed under normal use conditions.

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits

are exceeded or if irritation or other symptoms are experienced **Recommended Filter type:** Particulates filter conforming to EN 143

Small scale/Laboratory use Maintain adequate ventilation Use a NIOSH/MSHA or European Standard EN 149:2001

approved respirator if exposure limits are exceeded or if irritation or other symptoms are

experienced.

Recommended half mask:- Particle filtering: EN149:2001

Environmental exposure controls Prevent product from entering drains. Do not allow material to contaminate ground water

system. Local authorities should be advised if significant spillages cannot be contained.

Solid

Method - No information available

# **SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES**

## 9.1. Information on basic physical and chemical properties

Physical State Powder Solid

Appearance White Odor Slight

Odor ThresholdNo data availableMelting Point/Range230 °C / 446 °FSoftening PointNo data availableBoiling Point/RangeNo information available

Flammability (liquid) Not applicable

Flammability (solid,gas) No information available

Explosion Limits No data available

Flash Point No information available °C / °F

Autoignition Temperature 290 °C / 554 °F

Decomposition Temperature > 230°C

pH 5-7 @ 20°C (10 g/l aq.sol) Viscosity Not applicable Solid

Viscosity Not applicable S
Water Solubility 13 g/L (20°C)

Solubility in other solvents No information available

Partition Coefficient (n-octanol/water)

Component log Pow Hexadecyltrimethylammonium bromide 3.2 Vapor Pressure negligible

Density / Specific Gravity

No data available

Bulk Density

No data available

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#### (1-Hexadecyl)trimethylammonium bromide

Vapor Density Not applicable Solid

Particle characteristics No data available

9.2. Other information

Molecular Formula C19 H42 Br N Molecular Weight 364.45

Evaporation Rate Not applicable - Solid

# **SECTION 10: STABILITY AND REACTIVITY**

10.1. Reactivity

None known, based on information available

10.2. Chemical stability

Hygroscopic.

10.3. Possibility of hazardous reactions

**Hazardous Polymerization Hazardous Reactions**No information available.
None under normal processing.

10.4. Conditions to avoid

Avoid dust formation. Incompatible products. Excess heat. Exposure to moisture. Exposure

to moist air or water.

10.5. Incompatible materials

Strong oxidizing agents. Strong bases.

10.6. Hazardous decomposition products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen halides.

# **SECTION 11: TOXICOLOGICAL INFORMATION**

## 11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

## **Product Information**

(a) acute toxicity;

OralCategory 4DermalNo data availableInhalationNo data available

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Hexadecyltrimethylammonium bromide	LD50 = 410 mg/kg (Rat)	-	-

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 1

(d) respiratory or skin sensitization;

Respiratory No data available Skin No data available

## (1-Hexadecyl)trimethylammonium bromide

(e) germ cell mutagenicity; No data available

Not mutagenic in AMES Test

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; Category 3

Respiratory system. Results / Target organs

(i) STOT-repeated exposure; Category 2

Route of exposure

Gastrointestinal tract (GI). **Target Organs** 

Oral

(j) aspiration hazard; Solid

Not applicable

Symptoms / effects,both acute and No information available.

delayed

11.2. Information on other hazards

**Endocrine Disrupting Properties** Assess endocrine disrupting properties for human health. This product does not contain any

known or suspected endocrine disruptors.

# **SECTION 12: ECOLOGICAL INFORMATION**

12.1. Toxicity

**Ecotoxicity effects** The product contains following substances which are hazardous for the environment. Very

toxic to aquatic organisms, may cause long-term adverse effects in the aquatic

environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae
Hexadecyltrimethylammonium bromide			EC50: = 0.09 mg/L, 96h
			(Pseudokirchneriella subcapitata)

Component	Microtox	M-Factor
Hexadecyltrimethylammonium bromide	= 9.84 mg/L EC50 Photobacterium phosphoreum 5	10
	min	

12.2. Persistence and degradability Readily biodegradable

**Persistence** Persistence is unlikely.

Degradation in sewage Contains substances known to be hazardous to the environment or not degradable in waste

water treatment plants. treatment plant

12.3. Bioaccumulative potential Bioaccumulation is unlikely

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## (1-Hexadecyl)trimethylammonium bromide

Component	log Pow	Bioconcentration factor (BCF)
Hexadecyltrimethylammonium bromide	3.2	No data available

12.4. Mobility in soil The product is water soluble, and may spread in water systems. Will likely be mobile in the

environment due to its water solubility. Highly mobile in soils

12.5. Results of PBT and vPvB

assessment

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent

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and very bioaccumulative (vPvB).

12.6. Endocrine disrupting

properties

**Endocrine Disruptor Information** 

This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects

**Persistent Organic Pollutant Ozone Depletion Potential** 

This product does not contain any known or suspected substance This product does not contain any known or suspected substance

# SECTION 13: DISPOSAL CONSIDERATIONS

#### 13.1. Waste treatment methods

Waste from Residues/Unused

**Products** 

Should not be released into the environment. Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in

accordance with local regulations.

**Contaminated Packaging** Dispose of this container to hazardous or special waste collection point.

According to the European Waste Catalog, Waste Codes are not product specific, but **European Waste Catalogue (EWC)** 

application specific.

Other Information Do not flush to sewer. Waste codes should be assigned by the user based on the

application for which the product was used. Do not empty into drains. Do not let this

chemical enter the environment.

# **SECTION 14: TRANSPORT INFORMATION**

#### IMDG/IMO

14.1. UN number UN3077

ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. 14.2. UN proper shipping name

**Technical Shipping Name** Cetyltrimethylammonium bromide

14.3. Transport hazard class(es)

14.4. Packing group

Ш

**ADR** 

14.1. UN number UN3077

14.2. UN proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

**Technical Shipping Name** Cetyltrimethylammonium bromide

14.3. Transport hazard class(es) 9

14.4. Packing group Ш

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## (1-Hexadecyl)trimethylammonium bromide

#### IATA

**14.1. UN number** UN3077

14.2. UN proper shipping name ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.

Technical Shipping Name Cetyltrimethylammonium bromide

14.3. Transport hazard class(es) 9
14.4. Packing group III

**14.5. Environmental hazards** Dangerous for the environment

Product is a marine pollutant according to the criteria set by IMDG/IMO

14.6. Special precautions for user No special precautions required

14.7. Maritime transport in bulk according to IMO instruments

Not applicable, packaged goods

# **SECTION 15: REGULATORY INFORMATION**

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

## **International Inventories**

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Hexadecyltrimethylammonium	57-09-0	200-311-3	•	-	Х	Х	KE-34534	Χ	Χ
bromide									

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Hexadecyltrimethylammonium bromide	57-09-0	X	ACTIVE	X	-	X	X	Х

Legend: X - Listed '-' - Not Listed KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

# Authorisation/Restrictions according to EU REACH

Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization		REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Hexadecyltrimethylammonium bromide	57-09-0	-	-	-

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
Hexadecyltrimethylammoniu m bromide	57-09-0	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

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#### **National Regulations**

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

**WGK Classification** See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Hexadecyltrimethylammonium	WGK3	
bromide		

Component	Switzerland - Ordinance on the Reduction of Risk from handling of hazardous substances preparation (SR 814.81)	Switzerland - Ordinance on Incentive Taxes on Volatile Organic Compounds (OVOC)	Switzerland - Ordinance of the Rotterdam Convention on the Prior Informed Consent Procedure
Hexadecyltrimethylammonium bromide 57-09-0 ( <=100 )	Prohibited and Restricted Substances		

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

# **SECTION 16: OTHER INFORMATION**

## Full text of H-Statements referred to under sections 2 and 3

H302 - Harmful if swallowed

H315 - Causes skin irritation

H318 - Causes serious eye damage

H335 - May cause respiratory irritation

H373 - May cause damage to organs through prolonged or repeated exposure

H400 - Very toxic to aquatic life

H410 - Very toxic to aquatic life with long lasting effects

# Legend

**CAS** - Chemical Abstracts Service

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic

Substances/EU List of Notified Chemical Substances PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances **KECL** - Korean Existing and Evaluated Chemical Substances Substances List

**ENCS** - Japanese Existing and New Chemical Substances AICS - Australian Inventory of Chemical Substances NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level **RPE** - Respiratory Protective Equipment

LC50 - Lethal Concentration 50% NOEC - No Observed Effect Concentration PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50% POW - Partition coefficient Octanol:Water vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

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#### (1-Hexadecyl)trimethylammonium bromide

MARPOL - International Convention for the Prevention of Pollution from

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Ships

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

Dangerous Goods Code

ATE - Acute Toxicity Estimate
VOC - (Volatile Organic Compound)

Key literature references and sources for data

https://echa.europa.eu/information-on-chemicals

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Training Advice** 

Chemical incident response training.

Prepared By Health, Safety and Environmental Department

Creation Date02-Oct-2009Revision Date28-Jul-2022

**Revision Summary** SDS sections updated.

This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006. COMMISSION REGULATION (EU) 2020/878 amending Annex II to Regulation (EC) No. 1907/2006

**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 Safety Data Sheet**

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