
SECTION 1: Identification

1.1 GHS Product identifier

Product name Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine

1.2 Other means of identification

Product number -

Other names Oktogen; HW 4; 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane

1.3 Recommended use of the chemical and restrictions on use

Identified uses Propellants and blowing agents

Uses advised against no data available

SECTION 2: Hazard identification

2.1 Classification of the substance or mixture

Acute toxicity - Category 4, Oral

Acute toxicity - Category 3, Dermal

2.2 GHS label elements, including precautionary statements

Pictogram(s)



Signal word Danger

Hazard statement(s) H201 Explosive; mass explosion hazard

H302 Harmful if swallowed

H311 Toxic in contact with skin

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P316 Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P361+P364 Take off immediately all contaminated clothing and wash it before reuse.

Storage

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

2.3 Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	2691-41-0	220-260-0	100%

SECTION 4: First-aid measures

4.1 Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Refer for medical attention .

4.2 Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 112 [Explosives* - Division 1.1, 1.2, 1.3 or 1.5]: Fire may produce irritating, corrosive and/or toxic gases. (ERG, 2016)

4.3 Indication of immediate medical attention and special treatment needed, if necessary

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for pulmonary edema and treat if necessary . Monitor for shock and treat if necessary . Anticipate seizures and treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patient can swallow, has a strong gag reflex, and does not drool . Explosives

SECTION 5: Fire-fighting measures

5.1 Suitable extinguishing media

Evacuation: If the material is on fire or involved in fire consider evacuation of one (1) mile radius.

5.2 Specific hazards arising from the chemical

Excerpt from ERG Guide 112 [Explosives* - Division 1.1, 1.2, 1.3 or 1.5]: MAY EXPLODE AND THROW FRAGMENTS 1600 METERS (1 MILE) OR MORE IF FIRE REACHES CARGO. For information on "Compatibility Group" letters, refer to Glossary section. (ERG, 2016)

5.3 Special protective actions for fire-fighters

In case of fire in the surroundings, use appropriate extinguishing media. Combat fire from a sheltered position.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Consult an expert! Remove all ignition sources. Personal protection: chemical protection suit. Cover the spilled material with water. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT wash away into sewer. Do NOT let this chemical enter the environment.

6.2 Environmental precautions

Evacuate danger area! Consult an expert! Remove all ignition sources. Personal protection: chemical protection suit. Cover the spilled material with water. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT wash away into sewer. Do NOT let this chemical enter the environment.

6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

NO open flames, NO sparks and NO smoking. Closed system, ventilation, explosion-proof electrical equipment and lighting. Do NOT expose to friction or shock. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

7.2 Conditions for safe storage, including any incompatibilities

Fireproof. Separated from strong bases and strong acids. Store in an area without drain or sewer access.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational Exposure limit values

Component	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine			
CAS No.	2691-41-0			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m ³	ppm	mg/m ³
People's Republic of China		2		4 (1)
Remarks				
People's Republic of China	(1) 15 minutes average value			

Biological limit values

no data available

8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

8.3 Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety spectacles or eye protection in combination with breathing protection if powder.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation (not if powder), local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state	Cyclotetramethylene tetranitramine, [wet with $\geq 10\%$ water] is a white crystalline solid. Melting point 281°C . Practically insoluble in water. Water slurry mitigates explosion hazard. Used in solid propellants and explosives. The primary hazard is the blast effect and not flying projectiles and fragments.
Colour	White crystalline solid
Odour	no data available
Melting point/freezing point	286°C
Boiling point or initial boiling point and boiling range	906.1°C
Flammability	Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	501.8°C
Auto-ignition temperature	234°C
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water = 1.40×10^{-2} mg/L at 83°C
Partition coefficient n-octanol/water	$\log K_{ow} = 0.16$
Vapour pressure	2.07×10^{-32} mmHg at 25°C
Density and/or relative density	1.95 g/cm^3
Relative vapour density	no data available
Particle characteristics	no data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Heating may cause violent combustion or explosion. May decompose explosively on shock, friction or concussion. Decomposes on heating. This produces toxic gases including nitrogen oxides. Reacts violently with acids and bases.

10.2 Chemical stability

Stability at 300°K $\beta > \alpha > \gamma > \delta$. Beta is stable at room temp; alpha at $115\text{--}156^{\circ}\text{C}$; gamma at 156°C ; delta at /approximately/ $170\text{--}279^{\circ}\text{C}$.

10.3 Possibility of hazardous reactions

As a result of flow, agitation, etc., electrostatic charges can be generated. Dust explosion possible if in powder or granular form, mixed with air. CYCLOTETRAMETHYLENE TETRANITRAMINE, [WET WITH $\geq 10\%$ WATER] is a high explosive. May begin a vigorous reaction that culminates in a detonation if mixed with reducing agents, including hydrides, sulfides and nitrides. May explode in the presence of a base such as sodium hydroxide or potassium hydroxide even in the presence of water. Presence of metal oxides increases thermal sensitivity. Wetting reduces sensitivity toward detonation.

10.4 Conditions to avoid

no data available

10.5 Incompatible materials

no data available

10.6 Hazardous decomposition products

Decomposes violently at 279°C

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Mouse oral 1500 mg/kg
- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

CLASSIFICATION: D; not classifiable as to human carcinogenicity. BASIS FOR CLASSIFICATION: No cancer bioassays or epidemiological studies are available. HUMAN CARCINOGENICITY DATA: None.

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes and skin. The substance may cause effects on the central nervous system. This may result in irritability, convulsions and lowering of consciousness. Medical observation is indicated.

STOT-repeated exposure

The substance may have effects on the kidneys and liver.

Aspiration hazard

A harmful concentration of airborne particles can be reached quickly when dispersed.

SECTION 12: Ecological information

12.1 Toxicity

- Toxicity to fish: LC50 Pimephales promelas (Fathead minnow, 7-day old) 15 mg/L/96 hr; static /formulated product
- Toxicity to daphnia and other aquatic invertebrates: LC50 Daphnia magna (Water flea; intoxication, immobilization) >32 mg/L/24, 48 hr; static /formulated product
- Toxicity to algae: no data available
- Toxicity to microorganisms: no data available

12.2 Persistence and degradability

AEROBIC: Cyclotetramethylenetetranitramine has been reported to be resistant to biodegradation under aerobic conditions(1,2,3,4). No loss of cyclotetramethylenetetranitramine was observed in either fortified or field contaminated soil samples after 56 days during an aerobic biodegradation study(5). Cyclotetramethylenetetranitramine (22 mg/L) was not biodegraded aerobically after 28 days using a sludge enrichment culture from a sewage treatment plant(6). Bioremediation studies have reported that aerobic biodegradation of cyclotetramethylenetetranitramine is possible under specific conditions. Degradation of cyclotetramethylenetetranitramine was studied in water samples from the Holston River near the Holston Army Ammunition Plant in Kingsport, TN(7,8). Samples were collected downstream from a wasteline where this substance has been historically released. Cyclotetramethylenetetranitramine was not degraded aerobically after 15 days in the river water alone(7). However, when 50 ppm sterile yeast extract was added, the concentration decreased from 4 ppm to less than 0.1 ppm after three days of incubation(7). It was noted that degradation took place only in fresh samples and was not observed in stored river water. In a separate study, the biodegradation of cyclotetramethylenetetranitramine in dextrose, molasses, alfalfa, livestock manure, and in historically contaminated soil ranged from none to a reduction in concentration from 6 to 1 mg/L(9). Horse manure was reported to be the most successful regime(9). The biodegradability of cyclotetramethylenetetranitramine in an activated sludge unit, 5 days retention time, has been reported to be 53%(10).

12.3 Bioaccumulative potential

An estimated BCF of 1 was calculated for cyclotetramethylenetetranitramine(SRC), using a log Kow of 0.16(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC)

12.4 Mobility in soil

Experimentally determined Koc values for cyclotetramethylenetetranitramine in an agricultural topsoil and in Sasifrass sandy loam were 30 and 209, respectively(1). According to a classification scheme(2), Koc values ranging from 30-290 suggest that cyclotetramethylenetetranitramine is expected to have very high to moderate mobility in soil. A Koc value of 670 was determined for this chemical in Holston River sediment based on a measured sorption coefficient of 8.7 and an organic carbon content of 1.3%(3).

12.5 Other adverse effects

no data available

SECTION 13: Disposal considerations

13.1 Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

14.1 UN Number

ADR/RID: UN0484 (For reference only, please check.) IMDG: UN0484 (For reference only, please check.) IATA: UN0484 (For reference only, please check.)

14.2 UN Proper Shipping Name

ADR/RID: CYCLOTETRAMETHYLENE-TETRANITRAMINE (HMX; OCTOGEN), DESENSITIZED (For reference only, please check.) IMDG: CYCLOTETRAMETHYLENE-TETRANITRAMINE (HMX; OCTOGEN), DESENSITIZED (For reference only, please check.) IATA: CYCLOTETRAMETHYLENE-TETRANITRAMINE (HMX; OCTOGEN), DESENSITIZED (For reference only, please check.)

14.3 Transport hazard class(es)

ADR/RID: 1.1D (For reference only, please check.) IMDG: 1.1D (For reference only, please check.) IATA: 1.1D (For reference only, please check.)

14.4 Packing group, if applicable

ADR/RID: (For reference only, please check.) IMDG: (For reference only, please check.) IATA: (For reference only, please check.)

14.5 Environmental hazards

ADR/RID: No IMDG: No IATA: No

14.6 Special precautions for user

no data available

14.7 Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	2691-41-0	220-260-0
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Not Listed.
Vietnam National Chemical Inventory			Not Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Not Listed.

SECTION 16: Other information

Information on revision

Creation Date July 15, 2019
Revision Date July 15, 2019

Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Other Information

Combustion in a confined space may turn into detonation. The substance may be transported only in water (15%) or desensitized with wax.