# SAFETY DATA SHEET

Version 5.4
Revision Date 07/27/2018
Print Date 10/18/2018

## 1. PRODUCT AND COMPANY IDENTIFICATION

### 1.1 Product identifiers

Product name : (±)-threo-Methylphenidate-D4 HCl

Product Number : M-185
Brand : Cerilliant

### 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
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

### 1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

## 2. HAZARDS IDENTIFICATION

### 2.1 Classification of the substance or mixture

**GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**
Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 3), H301
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Specific target organ toxicity - single exposure (Category 1), H370

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

### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word Danger

Hazard statement(s)

| | |
|---|---|
| H225 | Highly flammable liquid and vapour. |
| H301 + H311 + H331 | Toxic if swallowed, in contact with skin or if inhaled. |
| H370 | Causes damage to organs. |

Precautionary statement(s)

| | |
|---|---|
| P210 | Keep away from heat/sparks/open flames/hot surfaces. No smoking. |
| P233 | Keep container tightly closed. |
| P240 | Ground/bond container and receiving equipment. |
| P241 | Use explosion-proof electrical/ ventilating/ lighting/ equipment. |
| P242 | Use only non-sparking tools. |
| P243 | Take precautionary measures against static discharge. |
| P260 | Do not breathe dust/ fume/ gas/ mist/ vapours/ spray. |

| | |
|---|---|
| P264 | Wash skin thoroughly after handling. |
| P270 | Do not eat, drink or smoke when using this product. |
| P271 | Use only outdoors or in a well-ventilated area. |
| P280 | Wear protective gloves/ protective clothing/ eye protection/ face protection. |
| P301 + P310 + P330 | IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth. |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower. |
| P304 + P340 + P311 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor. |
| P307 + P311 | IF exposed: Call a POISON CENTER or doctor/ physician. |
| P362 | Take off contaminated clothing and wash before reuse. |
| P370 + P378 | In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish. |
| P403 + P233 | Store in a well-ventilated place. Keep container tightly closed. |
| P403 + P235 | Store in a well-ventilated place. Keep cool. |
| P405 | Store locked up. |
| P501 | Dispose of contents/ container to an approved waste disposal plant. |

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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

Molecular weight : 32.04 g/mol

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

## 4. FIRST AID MEASURES

### 4.1 Description of first aid measures

**General advice**
Consult a physician. Show this safety data sheet to the doctor in attendance.Move out of dangerous area.

**If inhaled**
If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**
Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

**In case of eye contact**
Flush eyes with water as a precaution.

**If swallowed**
Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

## 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

No data available

### 5.3 Advice for firefighters
Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information
Use water spray to cool unopened containers.

## 6. ACCIDENTAL RELEASE MEASURES

### 6.1 Personal precautions, protective equipment and emergency procedures
Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.
For personal protection see section 8.

### 6.2 Environmental precautions
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up
Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

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

## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
Use explosion-proof equipment.Keep away from sources of ignition - No smoking.Take measures to prevent the build up of electrostatic charge.
For precautions see section 2.2.

### 7.2 Conditions for safe storage, including any incompatibilities
Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Recommended storage temperature -20 °C
Storage class (TRGS 510): 3: Flammable liquids

### 7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

**Components with workplace control parameters**

| Component | CAS-No. | Value | Control parameters | Basis |
|---|---|---|---|---|
| Methanol | 67-56-1 | TWA | 200 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Headache<br>Nausea<br>Dizziness<br>Eye damage<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section)<br>Danger of cutaneous absorption | | |
| | | STEL | 250 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | | Headache<br>Nausea<br>Dizziness<br>Eye damage<br>Substances for which there is a Biological Exposure Index or Indices (see BEI® section) | | |

| | | | | |
|---|---|---|---|---|
| | | Danger of cutaneous absorption | | |
| | | TWA | 200 ppm<br>260 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |
| | | ST | 250 ppm<br>325 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | Potential for dermal absorption | | |
| | | TWA | 200 ppm<br>260 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | The value in mg/m3 is approximate. | | |
| | | C | 1,000 ppm | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | PEL | 200 ppm<br>260 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | STEL | 250 ppm<br>325 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |

**Biological occupational exposure limits**

| Component | CAS-No. | Parameters | Value | Biological specimen | Basis |
|---|---|---|---|---|---|
| | - | Methanol | 15 mg/l | Urine | ACGIH - Biological Exposure Indices (BEI) |
| | Remarks | End of shift (As soon as possible after exposure ceases) | | | |

## 8.2 Exposure controls

**Appropriate engineering controls**
Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

**Personal protective equipment**

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

**Skin protection**
Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

**Body Protection**
Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory protection**
Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type AXBEK (EN 14387) 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**
Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## 9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

| | | |
|---|---|---|
| a) | Appearance | Form: liquid<br>Colour: colourless |
| b) | Odour | pungent |
| c) | Odour Threshold | No data available |
| d) | pH | No data available |
| e) | Melting point/freezing point | Melting point/range: -97.99 °C (-144.38 °F) |
| f) | Initial boiling point and boiling range | 64.0 - 65.0 °C (147.2 - 149.0 °F) at 1,013 hPa (760 mmHg) |
| g) | Flash point | No data available |
| h) | Evaporation rate | No data available |
| i) | Flammability (solid, gas) | No data available |
| j) | Upper/lower flammability or explosive limits | Upper explosion limit: 36 %(V)<br>Lower explosion limit: 6 %(V) |
| k) | Vapour pressure | 130.3 hPa (97.7 mmHg) at 20.0 °C (68.0 °F)<br>546.6 hPa (410.0 mmHg) at 50.0 °C (122.0 °F)<br>169.27 hPa (126.96 mmHg) at 25.0 °C (77.0 °F) |
| l) | Vapour density | 1.11 |
| m) | Relative density | 0.79 g/cm3 at 20 °C (68 °F) |
| n) | Water solubility | completely miscible |
| o) | Partition coefficient: n-octanol/water | log Pow: -0.769 |
| p) | Auto-ignition temperature | 455.0 °C (851.0 °F) at 1,013 hPa (760 mmHg) |
| q) | Decomposition temperature | No data available |
| r) | Viscosity | No data available |
| s) | Explosive properties | Not explosive |
| t) | Oxidizing properties | The substance or mixture is not classified as oxidizing. |

**9.2 Other safety information**

| | |
|---|---|
| Minimum ignition energy | 0.14 mJ |
| Conductivity | < 1 µS/cm |
| Relative vapour density | 1.11 |

## 10. STABILITY AND REACTIVITY

**10.1 Reactivity**
No data available

**10.2 Chemical stability**
Stable under recommended storage conditions.

**10.3 Possibility of hazardous reactions**
No data available

**10.4 Conditions to avoid**
Heat, flames and sparks.

**10.5 Incompatible materials**
Acid chlorides, Acid anhydrides, Oxidizing agents, Alkali metals, Reducing agents, Acids

**10.6 Hazardous decomposition products**
Hazardous decomposition products formed under fire conditions. - Carbon oxides
In the event of fire: see section 5

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

**Acute toxicity**
No data available

LD50 Oral - Rat - male and female - > 1,187 - 2,769 mg/kg
Remarks: (ECHA) (Regulation (EC) No 1272/2008, Annex VI)

LDLO Oral - Human - 143 mg/kg
Remarks: Lungs, Thorax, or Respiration:Dyspnea. Ingestion may cause gastrointestinal irritation, nausea, vomiting and diarrhoea.

Inhalation: No data available

LC50 Inhalation - Rat - male and female - 4 h - 131.25 mg/l
Remarks: (ECHA) (Regulation (EC) No 1272/2008, Annex VI)

Dermal: No data available

LD50 Dermal - Rabbit - 17,100 mg/kg
Remarks: (External MSDS) (Regulation (EC) No 1272/2008, Annex VI)

No data available

No data available

**Skin corrosion/irritation**
No data available

Skin - Rabbit
Result: No skin irritation
Remarks: (ECHA) Drying-out effect resulting in rough and chapped skin.

**Serious eye damage/eye irritation**
No data available

Eyes - Rabbit
Result: No eye irritation
Remarks: (ECHA) Irritation of mucous membranes

**Respiratory or skin sensitisation**
No data available

Maximisation Test - Guinea pig
Result: negative
(OECD Test Guideline 406)

**Germ cell mutagenicity**
No data available

Based on available data the classification criteria are not met.

Ames test
S. typhimurium
Result: negative

In vitro mammalian cell gene mutation test
fibroblast
Result: negative

OECD Test Guideline 474
Mouse - male and female - Bone marrow

Result: negative

**Carcinogenicity**

Did not show carcinogenic effects in animal experiments.

| | |
|---|---|
| IARC: | No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC. |
| ACGIH: | No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH. |
| NTP: | No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP. |
| OSHA: | No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens. |

**Reproductive toxicity**
No data available
No data available

Based on available data the classification criteria are not met.

**Specific target organ toxicity - single exposure**
No data available
Acute inhalation toxicity - Irritation symptoms in the respiratory tract.

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
No data available

**Additional Information**

| | |
|---|---|
| Repeated dose toxicity | Rat - male and female - Inhalation - 28 d - NOAEL : 6.66 mg/l - OECD Test Guideline 412 -Subacute toxicity |
| | Rat - male and female - Inhalation - 365 d - NOAEL : 0.13 mg/l - LOAEL : 1.3 mg/l - OECD Test Guideline 453 |

RTECS: Not available

Methyl alcohol may be fatal or cause blindness if swallowed.
Effects due to ingestion may include:, Headache, Dizziness, Drowsiness, metabolic acidosis, Coma, Seizures.
Symptoms may be delayed., Damage of the:, Liver, Kidney

Headache, Dizziness, Drowsiness, Coma, narcosis, Blindness, Impairment of vision, irritant effects, Nausea, Vomiting, agitation, spasms, inebriation
Drying-out effect resulting in rough and chapped skin., To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

## 12. ECOLOGICAL INFORMATION

### 12.1 Toxicity

No data available

| | |
|---|---|
| Toxicity to fish | flow-through test LC50 - Lepomis macrochirus (Bluegill) - 15,400.0 mg/l - 96 h (US-EPA) |
| Toxicity to daphnia and other aquatic invertebrates | EC50 - Daphnia magna (Water flea) - > 10,000 mg/l - 48 h<br>Remarks: (ECHA) |
| | semi-static test EC50 - Daphnia magna (Water flea) - 18,260 mg/l - 96 h (OECD Test Guideline 202) |
| Toxicity to algae | static test ErC50 - Pseudokirchneriella subcapitata (green algae) - ca. 22,000.0 mg/l - 96 h |

| | |
|---|---|
| | (OECD Test Guideline 201) |
| Toxicity to bacteria | EC5 - Pseudomonas fluorescens - 6,600 mg/l - 16 h<br>Remarks: (IUCLID) |
| | static test IC50 - activated sludge - > 1,000 mg/l - 3 h<br>(OECD Test Guideline 209) |

12.2 Persistence and degradability
No data available

| | |
|---|---|
| Biochemical Oxygen Demand (BOD) | 600 - 1,120 mg/g<br>Remarks: (IUCLID) |
| Chemical Oxygen Demand (COD) | 1,420 mg/g<br>Remarks: (IUCLID) |
| Theoretical oxygen demand | 1,500 mg/g<br>Remarks: (Lit.) |
| Ratio BOD/ThBOD | 76 %<br>Remarks: Closed Bottle test(IUCLID) |

**12.3 Bioaccumulative potential**
No data available

**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 Other adverse effects**
No data available

| | |
|---|---|
| Additional ecological information | Avoid release to the environment. |
| Stability in water | at 19 °C83 - 91 % - 72 h<br>Remarks: Hydrolyses on contact with water.Hydrolyses readily. |

## 13. DISPOSAL CONSIDERATIONS

**13.1 Waste treatment methods**

**Product**
Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**
Dispose of as unused product.

## 14. TRANSPORT INFORMATION

**DOT (US)**
UN number: 1230 Class: 3 Packing group: II
Proper shipping name: Methanol, solution
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

**IMDG**
UN number: 1230 Class: 3 (6.1) Packing group: II EMS-No: F-E, S-D
Proper shipping name: METHANOL, SOLUTION

**IATA**
UN number: 1230 Class: 3 (6.1) Packing group: II

Proper shipping name: Methanol, solution

## 15. REGULATORY INFORMATION

**SARA 302 Components**
No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**
The following components are subject to reporting levels established by SARA Title III, Section 313:

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |

**SARA 311/312 Hazards**
Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |

**Pennsylvania Right To Know Components**

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |

**New Jersey Right To Know Components**

| | CAS-No. | Revision Date |
|---|---|---|
| Methanol | 67-56-1 | 2007-07-01 |

**California Prop. 65 Components**

| | CAS-No. | Revision Date |
|---|---|---|
| WARNING: This product contains a chemical known to the State of California to cause birth defects or other reproductive harm.<br>Methanol | 67-56-1 | 2012-03-16 |

## 16. OTHER INFORMATION

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

| | |
|---|---|
| H225 | Highly flammable liquid and vapour. |
| H301 | Toxic if swallowed. |
| H311 | Toxic in contact with skin. |
| H331 | Toxic if inhaled. |
| H370 | Causes damage to organs. |

Further information
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**Preparation Information**
Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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