Acetonitrile-d3 (for NMR Spectroscopy) **CAS No 2206-26-0**	**MATERIAL SAFETY DATA SHEET SDS/MSDS**

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

1.1 Product identifiers

Product name : **Acetonitrile**-d3 (for NMR Spectroscopy)

CAS-No. : 2206-26-0

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

Identified uses : Laboratory chemicals, Industrial & for professional use only.

1.3 Details of the supplier of the safety data sheet

Company : Central Drug House (P) Ltd
DGL 128-129, DLF The Galleria,
Mayur Vihar Phase 1 Extension,
New Delhi-110091
INDIA

Telephone : +91 11 49404040
Email : care@cdhfinechemical.com

1.4 Emergency telephone number

Emergency Phone # : +91 11 49404040 (9:00am - 6:00 pm) [Office hours]

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008
Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Eye irritation (Category 2), H319

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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008
Pictogram



Signal word Danger

Hazard statement(s)

H225	Highly flammable liquid and vapour.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled
H319	Causes serious eye irritation.

Precautionary statement(s)	
P210	Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280	Wear protective gloves/ protective clothing.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	:	Trideuteroacetonitrile Methyl-d3 cyanide
Formula	:	C2D3N
Molecular weight	:	44.08 g/mol
CAS-No.	:	2206-26-0
EC-No.	:	218-616-5

Hazardous ingredients according to Regulation (EC) No 1272/2008

Component		Classification	Concentration
Acetonitrile-d3			
CAS-No.	2206-26-0	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2; H225, H302, H332, H312, H319	<= 100 %
EC-No.	218-616-5		

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

SECTION 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.

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. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

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

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)

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.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures
Use personal protective equipment. 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.

SECTION 7: Handling and storage

7.1 Precautions for safe handling
Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.
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
Store in cool place. 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.

Handle and store under inert gas. hygroscopic
Storage class (TRGS 510): Flammable liquids

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

8.2 Exposure controls

Appropriate engineering controls
Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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 (US) or type ABEK (EN 14387) respirator cartridges as a backup to enginee 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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a)	Appearance	Form: clear, liquid Colour: colourless
b)	Odour	pungent
c)	Odour Threshold	No data available
d)	pH	No data available
e)	Melting point/freezing point	No data available
f)	Initial boiling point and boiling range	80.7 °C - lit.
g)	Flash point	2.00 °C - closed cup
h)	Evaporation rate	No data available
i)	Flammability (solid, gas)	No data available
j)	Upper/lower flammability or explosive limits	Upper explosion limit: 16.00 %(V) Lower explosion limit: 4.40 %(V)
k)	Vapour pressure	413.23 hPa at 55.00 °C 73.18 hPa at 15.00 °C 119.81 hPa at 25.00 °C
l)	Vapour density	No data available

m) Relative density	0.844 g/cm3 at 25 °C
n) Water solubility	soluble
o) Partition coefficient: n-octanol/water	log Pow: -0.339
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information
No data available

SECTION 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
acids, Bases, Oxidizing agents, Reducing agents, Alkali metals

10.6 Hazardous decomposition products
Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)
Other decomposition products - No data available
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Rat - 2,460 mg/kg(Acetonitrile-d3)
LC50 Inhalation - Rat - 8.00 h - 7551 ppm(Acetonitrile-d3)
Remarks: Behavioral:Altered sleep time (including change in righting reflex). Behavioral:Convulsions or effect on seizure threshold. Blood: Hemorrhage.
LD50 Dermal - Rabbit - 2,000 mg/kg(Acetonitrile-d3)

Skin corrosion/irritation
Skin - Rabbit(Acetonitrile-d3)
Result: Mild skin irritation

Serious eye damage/eye irritation
Eyes - Rabbit(Acetonitrile-d3)
Result: Irritating to eyes.

(OECD Test Guideline 405)

Respiratory or skin sensitisation
No data available(Acetonitrile-d3)

Germ cell mutagenicity

No data available(Acetonitrile-d3)

Carcinogenicity

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.

Reproductive toxicity
No data available(Acetonitrile-d3)

Specific target organ toxicity - single exposure
No data available(Acetonitrile-d3)

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available(Acetonitrile-d3)

Additional Information
RTECS: Not available

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhoea(Acetonitrile-d3)

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	LC50 - Pimephales promelas (fathead minnow) - 1,640 mg/l - 96.0 h(Acetonitrile-d3)

12.2 Persistence and degradability
No data available

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available(Acetonitrile-d3)

12.5 Results of PBT and vPvB assessment
This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Other adverse effects

No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product
Burn in a chemical incinerator equipped with an afterburner and scrubber b highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1648 IMDG: 1648 IATA: 1648

14.2 UN proper shipping name

ADR/RID: ACETONITRILE
IMDG: ACETONITRILE
IATA: Acetonitrile

14.3 Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

14.4 Packaging group

ADR/RID: II IMDG: II IATA: II

14.5 Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

14.6 Special precautions for user

No data available

SECTION 15: Regulatory information

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

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

15.2 Chemical safety assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

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

H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled
H312	Harmful in contact with skin.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

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. Central Drug House (P) Ltd and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.cdhfinechemical.com for additional terms and conditions of sale.