

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 19.11.2012

Version 7.0

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

1.1 Product identifier

Catalogue No. 815008

Product name Ammonia-D3 25% solution in D₂O deuteration degree min. 99.5% for NMR spectroscopy MagniSolv™

REACH Registration Number This product is a mixture. REACH Registration Number see section 3.

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

Identified uses Reagent for analysis

For additional information on uses please refer to the Merck Chemicals portal (www.merck-chemicals.com).

1.3 Details of the supplier of the safety data sheet

Company Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0

Responsible Department LS-QHC * e-mail: prodsafe@merckgroup.com

1.4 Emergency telephone number Please contact the regional company representation in your country.

SECTION 2. Hazards identification

2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

Corrosive to metals, Category 1, H290

Skin corrosion, Category 1B, H314

Specific target organ toxicity - single exposure, Category 3, H335

Acute aquatic toxicity, Category 1, H400

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

Classification (67/548/EEC or 1999/45/EC)

C	Corrosive	R34
N	Dangerous for the environment	R50

For the full text of the R-phrases mentioned in this Section, see Section 16.

2.2 Label elements

Labelling (REGULATION (EC) No 1272/2008)

Hazard pictograms



Signal word

Danger

Hazard statements

H290 May be corrosive to metals.

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H314 Causes severe skin burns and eye damage.
H335 May cause respiratory irritation.
H400 Very toxic to aquatic life.

Precautionary statements

Prevention

P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

Reduced labelling (≤125 ml)

Hazard pictograms



Signal word

Danger

Hazard statements

H314 Causes severe skin burns and eye damage.

Precautionary statements

P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331 IF SWALLOWED: rinse mouth. Do NOT induce vomiting.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P309 + P310 IF exposed or if you feel unwell: Immediately call a POISON CENTER or doctor/physician.

Labelling (67/548/EEC or 1999/45/EC)

<i>Symbol(s)</i>	C	Corrosive
	N	Dangerous for the environment
<i>R-phrases(s)</i>	34-50	Causes burns. Very toxic to aquatic organisms.
<i>S-phrases(s)</i>	26-36/37/39-45-61	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Avoid release to the environment. Refer to special instructions/ Safety data sheets.

Reduced labelling (≤125 ml)

<i>Symbol(s)</i>	C	Corrosive
	N	Dangerous for the environment
<i>R-phrases(s)</i>	34	Causes burns.
<i>S-phrases(s)</i>	26-36/37/39-45	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

2.3 Other hazards

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None known.

SECTION 3. Composition/information on ingredients

Chemical nature	Aqueous ammoniacal solution. (deuterated form)
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3.1 Substance
not applicable

3.2 Mixture

Formula	ND ₄ OD	D ₅ NO (Hill)
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Hazardous components (REGULATION (EC) No 1272/2008)

Chemical Name (Concentration)

CAS-No.	Registration number	Classification
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[²H₄]ammonium-[²H]hydroxide (>= 25 % - < 50 %)

12168-30-8 *)

Skin corrosion, Category 1B, H314

Corrosive to metals, Category 1, H290

Acute aquatic toxicity, Category 1, H400

Specific target organ toxicity - single exposure, Category 3, H335

*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

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

Hazardous components (1999/45/EC)

Chemical Name (Concentration)

CAS-No.	Classification
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[²H₄]ammonium-[²H]hydroxide (>= 25 % - < 50 %)

12168-30-8 C, Corrosive; R34

N, Dangerous for the environment; R50

For the full text of the R-phrases mentioned in this Section, see Section 16.

SECTION 4. First aid measures

4.1 Description of first aid measures

After inhalation: fresh air. Call in physician.

After skin contact: wash off with plenty of water. Immediately remove contaminated clothing. If available swab with polyethylene glycol 400. Call a physician immediately.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

Irritation and corrosion, bronchitis, Cough, Shortness of breath, gastric pain, Unconsciousness, Bloody vomiting, Nausea, collapse, shock
Risk of blindness!

4.3 Indication of any immediate medical attention and special treatment needed

No information available.

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SECTION 5. Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Not combustible.

Ammonia solution itself is not flammable, but can form an ignitable ammonia/air-mixture by outgassing.

Ambient fire may liberate hazardous vapours.

Fire may cause evolution of:
nitrogen oxides

5.3 Advice for firefighters

Special protective equipment 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.

Further information

Cool closed containers exposed to fire with water spray. Suppress (knock down) gases/vapours/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: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

6.2 Environmental precautions

Do not empty into 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 with liquid-absorbent and neutralising material (e.g. Chemisorb® OH⁻, Merck Art. No. 101596). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

Indications about waste treatment see section 13.

SECTION 7. Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Observe label precautions.

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Hygiene measures

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

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed.

Store at +15°C to +25°C.

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

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

Individual protection measures

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

Eye/face protection

Tightly fitting safety goggles

Hand protection

full contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 240 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

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).

Other protective equipment

protective clothing

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Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter K (acc. to DIN 3181) for NH₃

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

Environmental exposure controls

Do not empty into drains.

SECTION 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Form	liquid
Colour	colourless
Odour	stinging
Odour Threshold	0,03 - 0,05 ppm Ammonia
pH	at 20 °C strongly alkaline
Melting point	No information available.
Boiling point/boiling range	ca. 36 °C
Flash point	No information available.
Evaporation rate	No information available.
Flammability (solid, gas)	not applicable
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	535 hPa at 20 °C
Relative vapor density	No information available.
Relative density	1,056 g/cm ³ at 20 °C
Water solubility	at 20 °C soluble

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Partition coefficient: n-octanol/water	log Pow: -1,38 (experimental) (anhydrous substance) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	No information available.
Explosive properties	Not classified as explosive.
Oxidizing properties	none

9.2 Other data

Minimum ignition energy	380 - 680 mJ
Corrosion	May be corrosive to metals.

SECTION 10. Stability and reactivity

10.1 Reactivity

See section 10.3

10.2 Chemical stability

Ammonia solution itself is not flammable, but can form an ignitable ammonia/air-mixture by outgassing.

10.3 Possibility of hazardous reactions

A risk of explosion and/or of toxic gas formation exists with the following substances:

Oxidizing agents, Phosgene, Oxides of phosphorus, Mercury, acids, Nitric acid, Oxygen, sulphur dioxide, hydrogen sulphide, silver compounds, nitrogen oxides, nitrogen trichloride, hydrogen peroxide, silver, Lead, Zinc, Heavy metals, Heavy metal salts, strong alkalis, Acrolein, antimony hydride, Boron, hydrogen bromide, chlorates, Hydrogen chloride gas, chromium(VI) oxide, chromyl chloride, dimethylsulfate, Ethylene oxide, Hydrogen fluoride, halogens, halogen-halogen compounds, halogen oxides, carbon dioxide, Acids

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

Aluminium, Lead, Copper, various metals, metal alloys, Nickel, silver, Zinc

10.6 Hazardous decomposition products

in the event of fire: See section 5.

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SECTION 11. Toxicological information

11.1 Information on toxicological effects

Mixture

Acute oral toxicity

LDLO human: 43 mg/kg (29% solution) (RTECS)

Symptoms: gastric pain, Bloody vomiting, If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.

Acute inhalation toxicity

This information is not available.

Acute dermal toxicity

This information is not available.

Skin irritation

rabbit

Result: Severe irritations

(29% solution) (RTECS)

Dermatitis Necrosis

Mixture causes burns.

Eye irritation

rabbit

Result: Severe irritations

(29% solution) (RTECS)

Mixture causes serious eye damage. Risk of blindness!

Sensitisation

Sensitisation test: guinea pig

Result: negative

(anhydrous substance) (IUCLID)

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

(anhydrous substance) (IUCLID)

Ames test

Escherichia coli

Result: negative

(anhydrous substance) (IUCLID)

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

Mixture may cause respiratory irritation.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

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11.2 Further information

Systemic effects:

Nausea, collapse, shock, Shortness of breath, Unconsciousness

Further data:

Handle in accordance with good industrial hygiene and safety practice.

Components

[²H₄]ammonium-[²H]hydroxide

No information available.

SECTION 12. Ecological information

Mixture

12.1 Toxicity

Toxicity to fish

LC50 Oncorhynchus mykiss (rainbow trout): 0,53 mg/l; 96 h (anhydrous substance) (Lit.)

Toxicity to daphnia and other aquatic invertebrates

EC50 Daphnia magna (Water flea): 24 mg/l; 48 h (anhydrous substance) (Lit.)

Toxicity to bacteria

EC50 Photobacterium phosphoreum: 2 mg/l; 5 min (anhydrous substance) (Lit.)

12.2 Persistence and degradability

Biodegradability

Not readily biodegradable.

12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: -1,38

(experimental)

(anhydrous substance) Bioaccumulation is not expected.

12.4 Mobility in soil

No information 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

Additional ecological information

Biological effects:

Harmful effect due to pH shift.

Forms toxic mixtures in water, dilution measures notwithstanding.

Further information on ecology

Discharge into the environment must be avoided.

Components

[²H₄]ammonium-[²H]hydroxide

No information available.

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SECTION 13. Disposal considerations

Waste treatment methods

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14. Transport information

Land transport (ADR/RID)

14.1 UN number	UN 2672
14.2 Proper shipping name	AMMONIA SOLUTION
14.3 Class	8
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	yes
Tunnel restriction code	E

Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

14.1 UN number	UN 2672
14.2 Proper shipping name	AMMONIA SOLUTION
14.3 Class	8
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	no

Sea transport (IMDG)

14.1 UN number	UN 2672
14.2 Proper shipping name	AMMONIA SOLUTION
14.3 Class	8
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	yes
EmS	F-A S-B

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code
Not relevant

SECTION 15. Regulatory information

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

EU regulations

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Major Accident Hazard Legislation	96/82/EC Dangerous for the environment 9a Quantity 1: 100 t Quantity 2: 200 t
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Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
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National legislation

Storage class	8B
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15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out.

SECTION 16. Other information

Details in analogy to the undeuterated compound.

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

H290	May be corrosive to metals.
H314	Causes severe skin burns and eye damage.
H335	May cause respiratory irritation.
H400	Very toxic to aquatic life.

Full text of R-phrases referred to under sections 2 and 3

R34	Causes burns.
R50	Very toxic to aquatic organisms.

Training advice

Provide adequate information, instruction and training for operators.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Regional representation

This information is given on the authorised Safety Data Sheet for your country.

The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.