

SAFETY DATA SHEET



NMR Sample ID 2

Section 1. Identification

This product is considered an article. This Material Safety Data Sheet is written based on the encapsulated substance or mixture in this article.

1.1 Product identifier

Product name : NMR Sample ID 2
Part No. : 96812097, 96812397, 190350697, 190350897, 190835397, 190887097, 191120797
Validation date : 01/15/2014.

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

Material uses : Analytical chemistry.
860 µl (96812097)
3500 µl (96812397)
250 µl (190350697)
2100 µl (190350897)
450 µl (190835397)
42 µl (190636197, 190887097)
71 µl (191120797)

1.3 Details of the supplier of the safety data sheet

Supplier/Manufacturer : Agilent Technologies, Inc.
Logistics Center - Americas
500 Ships Landing Way
New Castle, Delaware 19720
800-227-9770

1.4 Emergency telephone number

In case of emergency : CHEMTREC®: 1-800-424-9300

Section 2. Hazards identification

This article, when used under reasonable conditions and in accordance with the directions for use, should not present a health hazard. The substance or mixture is encapsulated in the article. Only if released due to use or processing of the article in a manner not in accordance with the product's directions for use it may present potential health and safety hazards.

2.1 Classification of the substance or mixture

OSHA/HCS status : This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).

Classification of the substance or mixture

H227 FLAMMABLE LIQUIDS - Category 4
H320 SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2B
H373 SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2

2.2 GHS label elements

Hazard pictograms :

Signal word : Warning

Section 2. Hazards identification

- Hazard statements** : H227 - Combustible liquid.
H320 - Causes eye irritation.
H373 - May cause damage to organs through prolonged or repeated exposure.
- Precautionary statements**
- Prevention** : P280 - Wear protective gloves. Wear eye or face protection.
P210 - Keep away from flames and hot surfaces. - No smoking.
P260 - Do not breathe vapor.
P264 - Wash hands thoroughly after handling.
- Response** : P314 - Get medical attention if you feel unwell.
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313 - If eye irritation persists: Get medical attention.
- Storage** : P403 - Store in a well-ventilated place.
P235 - Keep cool.
- Disposal** : P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.

2.3 Other hazards

- Hazards not otherwise classified** : None known.

Section 3. Composition/information on ingredients

This article, when used under reasonable conditions and in accordance with the directions for use, should not present a health hazard. The substance or mixture is encapsulated in the article. Only if released due to use or processing of the article in a manner not in accordance with the product's directions for use it may present potential health and safety hazards.

- Substance/mixture** : Mixture

Ingredient name	%	CAS number
di[(² H ₃)Methyl] sulphoxide	60 - 100	2206-27-1
Benzamide (¹⁵ N)	1 - 5	31656-62-9

Any concentration shown as a range is to protect confidentiality or is due to batch variation.

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment and hence require reporting in this section.

Occupational exposure limits, if available, are listed in Section 8.

Section 4. First aid measures

4.1 Description of necessary first aid measures

- Eye contact** : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention following exposure or if feeling unwell.
- Inhalation** : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention following exposure or if feeling unwell. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.
- Skin contact** : Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Continue to rinse for at least 10 minutes. Get medical attention following exposure or if feeling unwell. Wash clothing before reuse. Clean shoes thoroughly before reuse.

Section 4. First aid measures

Ingestion : Wash out mouth with water. Remove dentures if any. Remove victim to fresh air and keep at rest in a position comfortable for breathing. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Stop if the exposed person feels sick as vomiting may be dangerous. Do not induce vomiting unless directed to do so by medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Get medical attention following exposure or if feeling unwell. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.

4.2 Most important symptoms/effects, acute and delayed

Potential acute health effects

Eye contact : Causes eye irritation.
Inhalation : No known significant effects or critical hazards.
Skin contact : No known significant effects or critical hazards.
Ingestion : May be irritating to mouth, throat and stomach.

Over-exposure signs/symptoms

Eye contact : Adverse symptoms may include the following:
 irritation
 watering
 redness

Inhalation : No specific data.
Skin contact : No specific data.
Ingestion : No specific data.

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

Notes to physician : Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.

Specific treatments : No specific treatment.

Protection of first-aiders : No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

See toxicological information (Section 11)

Section 5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media : Use dry chemical, CO₂, water spray (fog) or foam.

Unsuitable extinguishing media : Do not use water jet.

5.2 Special hazards arising from the substance or mixture

Specific hazards arising from the chemical : Combustible liquid. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. The vapor/gas is heavier than air and will spread along the ground. Vapors may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. Runoff to sewer may create fire or explosion hazard.

Hazardous thermal decomposition products : Decomposition products may include the following materials:
 carbon dioxide
 carbon monoxide
 sulfur oxides

Section 5. Fire-fighting measures

5.3 Advice for firefighters

- Special protective actions for fire-fighters** : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.
- Special protective equipment for fire-fighters** : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

- For non-emergency personnel** : No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
- For emergency responders** : If specialised clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

- 6.2 Environmental precautions** : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

6.3 Methods and materials for containment and cleaning up

Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Dilute with water and mop up if water-soluble. Alternatively, or if water-insoluble, absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.

Section 7. Handling and storage

7.1 Precautions for safe handling

- Protective measures** : Put on appropriate personal protective equipment (see Section 8). Do not breathe vapor or mist. Do not ingest. Avoid contact with eyes, skin and clothing. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use only non-sparking tools. Empty containers retain product residue and can be hazardous. Do not reuse container.
- Advice on general occupational hygiene** : Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

- 7.2 Conditions for safe storage, including any incompatibilities** : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination.

Section 7. Handling and storage

7.3 Specific end use(s)

Recommendations : Industrial applications, Professional applications.

Industrial sector specific solutions : Not applicable.

Section 8. Exposure controls/personal protection

Since the hazardous ingredient in this article is encapsulated, the risk of exposure by inhalation, ingestion, skin contact and eyes contact is minimum.

8.1 Control parameters

Occupational exposure limits

Ingredient name	Exposure limits
di[(² H ₃)Methyl] sulphoxide	AIHA WEEL (United States, 10/2011). TWA: 250 ppm 8 hours.

8.2 Exposure controls

Appropriate engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Environmental exposure controls : Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

Individual protection measures

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: chemical splash goggles.

Skin protection

Hand protection : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

Body protection : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Other skin protection : Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.

Section 8. Exposure controls/personal protection

- Respiratory protection** : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

Section 9. Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

- Physical state** : Liquid. [Clear.]
- Color** : Colorless.
- Odor** : Ripe olive.
- Odor threshold** : Not available.
- pH** : Not available.
- Melting point** : 18 to 18.54°C (64.4 to 65.4°F)
- Boiling point** : 189°C (372.2°F)
- Flash point** : Closed cup: 88°C (190.4°F)
- Evaporation rate** : Not available.
- Flammability (solid, gas)** : Not available.
- Lower and upper explosive (flammable) limits** : Lower: 3%
- Vapor pressure** : 0.061 kPa (0.46 mm Hg) [room temperature]
- Vapor density** : 1.04 [Air = 1]
- Relative density** : 1.18
- Solubility** : Soluble in the following materials: cold water and hot water.
- Solubility in water** : Not available.
- Partition coefficient: n-octanol/water** : Not available.
- Auto-ignition temperature** : 215°C (419°F)
- Decomposition temperature** : Not available.
- Viscosity** : Not available.

Section 10. Stability and reactivity

- 10.1 Reactivity** : No specific test data related to reactivity available for this product or its ingredients.
- 10.2 Chemical stability** : The product is stable.
- 10.3 Possibility of hazardous reactions** : Under normal conditions of storage and use, hazardous reactions will not occur.
- 10.4 Conditions to avoid** : Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition. Do not allow vapor to accumulate in low or confined areas.
- 10.5 Incompatible materials** : Reactive or incompatible with the following materials:
oxidizing materials
Absorbs moisture from the air.

Section 10. Stability and reactivity

10.6 Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Section 11. Toxicological information

11.1 Information on toxicological effects

Acute toxicity

Product/ingredient name	Result	Species	Dose	Exposure
di[(² H ₃)Methyl] sulphoxide	LD50 Dermal	Rat	40000 mg/kg	-
	LD50 Oral	Rat	14500 mg/kg	-

Irritation/Corrosion

Product/ingredient name	Result	Species	Score	Exposure	Observation
di[(² H ₃)Methyl] sulphoxide	Eyes - Mild irritant	Rabbit	-	24 hours 500 milligrams	-
	Eyes - Mild irritant	Rabbit	-	100 milligrams	-
	Skin - Mild irritant	Rabbit	-	24 hours 500 milligrams	-
	Skin - Mild irritant	Rabbit	-	100 milligrams	-

Sensitization

Not available.

Mutagenicity

Not available.

Carcinogenicity

Not available.

Reproductive toxicity

Not available.

Teratogenicity

Not available.

Specific target organ toxicity (single exposure)

Not available.

Specific target organ toxicity (repeated exposure)

Name	Category	Route of exposure	Target organs
di[(² H ₃)Methyl] sulphoxide	Category 2	Oral	kidneys and liver

Aspiration hazard

Not available.

Information on the likely routes of exposure : Not available.

Potential acute health effects

Eye contact : Causes eye irritation.

Inhalation : No known significant effects or critical hazards.

Skin contact : No known significant effects or critical hazards.

Section 11. Toxicological information

Ingestion : May be irritating to mouth, throat and stomach.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact : Adverse symptoms may include the following:
irritation
watering
redness

Inhalation : No specific data.

Skin contact : No specific data.

Ingestion : No specific data.

Delayed and immediate effects and also chronic effects from short and long term exposure

Short term exposure

Potential immediate effects : Not available.

Potential delayed effects : Not available.

Long term exposure

Potential immediate effects : Not available.

Potential delayed effects : Not available.

Potential chronic health effects

Not available.

General : May cause damage to organs through prolonged or repeated exposure.

Carcinogenicity : No known significant effects or critical hazards.

Mutagenicity : No known significant effects or critical hazards.

Teratogenicity : No known significant effects or critical hazards.

Developmental effects : No known significant effects or critical hazards.

Fertility effects : No known significant effects or critical hazards.

Numerical measures of toxicity

Acute toxicity estimates

Route	ATE value
Oral	25000 mg/kg

Section 12. Ecological information

12.1 Toxicity

Product/ingredient name	Result	Species	Exposure
di[(² H ₃)Methyl] sulphoxide	Acute LC50 25000 ppm Fresh water	Daphnia - Daphnia magna - Neonate	48 hours
Benzamide (¹⁵ N)	Acute LC50 34000000 µg/l Fresh water	Fish - Pimephales promelas	96 hours
	Acute LC50 661000 µg/l Fresh water	Fish - Pimephales promelas	96 hours

12.2 Persistence and degradability

Not available.

Section 12. Ecological information

12.3 Bioaccumulative potential

Product/ingredient name	LogP _{ow}	BCF	Potential
di[(² H ₃)Methyl] sulphoxide	-1.35	3.16	low

12.4 Mobility in soil

Soil/water partition coefficient (K_{oc}) : Not available.

12.5 Other adverse effects : No known significant effects or critical hazards.

Section 13. Disposal considerations

13.1 Waste treatment methods

Disposal methods : The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and its container must be disposed of in a safe way. Care should be taken when handling emptied containers that have not been cleaned or rinsed out. Empty containers or liners may retain some product residues. Vapor from product residues may create a highly flammable or explosive atmosphere inside the container. Do not cut, weld or grind used containers unless they have been cleaned thoroughly internally. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Disposal should be in accordance with applicable regional, national and local laws and regulations. Local regulations may be more stringent than regional or national requirements.

The information presented below only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations.

Refer to Section 7: HANDLING AND STORAGE and Section 8: EXPOSURE CONTROLS/PERSONAL PROTECTION for additional handling information and protection of employees.

Section 14. Transport information

This Material Safety Data Sheet is written based on the encapsulated substance or mixture in this article. Since the hazardous ingredient is encapsulated, the risk of exposure by inhalation, ingestion, skin contact and eyes contact is minimum.

Regulatory information

DOT / IMDG / IATA : Not regulated.

Section 15. Regulatory information

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

U.S. Federal regulations : **United States inventory (TSCA 8b)**: Not determined.
Clean Water Act (CWA) 307: Chromium(III) 4-oxopent-2-ene-2-olate

Clean Air Act Section 112 (b) Hazardous Air Pollutants (HAPs) : Not listed

Clean Air Act Section 602 Class I Substances : Not listed

Clean Air Act Section 602 Class II Substances : Not listed

DEA List I Chemicals (Precursor Chemicals) : Not listed

DEA List II Chemicals (Essential Chemicals) : Not listed

SARA 302/304

Composition/information on ingredients

No products were found.

SARA 304 RQ : Not applicable.

SARA 311/312

Classification : Fire hazard
 Immediate (acute) health hazard
 Delayed (chronic) health hazard

Composition/information on ingredients

Name	%	Fire hazard	Sudden release of pressure	Reactive	Immediate (acute) health hazard	Delayed (chronic) health hazard
di[(² H ₃)Methyl] sulphoxide Benzamide (¹⁵ N)	60 - 100 1 - 5	Yes. No.	No. No.	No. No.	Yes. Yes.	Yes. No.

SARA 313

	Product name	CAS number	%
Form R - Reporting requirements	Benzamide (¹⁵ N)	31656-62-9	1 - 5
Supplier notification	Benzamide (¹⁵ N)	31656-62-9	1 - 5

SARA 313 notifications must not be detached from the SDS and any copying and redistribution of the SDS shall include copying and redistribution of the notice attached to copies of the SDS subsequently redistributed.

State regulations

Massachusetts : None of the components are listed.

New York : None of the components are listed.

New Jersey : The following components are listed: DIMETHYL SULFOXIDE; METHANE, SULFINYLBI-

Pennsylvania : The following components are listed: di[(²H₃)Methyl] sulphoxide

California Prop. 65

No products were found.

Canada inventory : Not determined.

Section 15. Regulatory information

International regulations

International lists	: Australia inventory (AICS): Not determined. China inventory (IECSC): Not determined. Japan inventory: Not determined. Korea inventory: Not determined. Malaysia Inventory (EHS Register): Not determined. New Zealand Inventory of Chemicals (NZIoC): Not determined. Philippines inventory (PICCS): Not determined. Taiwan inventory (CSNN): Not determined.
Chemical Weapons Convention List Schedule I Chemicals	: Not listed
Chemical Weapons Convention List Schedule II Chemicals	: Not listed
Chemical Weapons Convention List Schedule III Chemicals	: Not listed

Section 16. Other information

History

Date of issue	: 01/15/2014.
Date of previous issue	: 10/16/2013.
Version	: 2.2

✔ Indicates information that has changed from previously issued version.

Notice to reader

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