

SAFETY DATA SHEET



3mm sample kit - cold probe 13C, Part Number 190350511

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 : 3mm sample kit - cold probe 13C, Part Number 190350511
Part No. (Chemical Kit) : 190350511
Part No. : 1H S/N 190350670
 4Hz 0.1% H2O/D2O 190350609
 Temp Grad 190350611
 1H Lineshape 190350689
 13C S/N ASTM doped 190350691
 ID 1 190350696
 ID 2 190350697
 Sucrose, NMR tested 190350612

Validation date : 29/01/2014.

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

Material uses : Analytical chemistry.
 1H S/N 250 µl
 4Hz 0.1% H2O/D2O 250 µl
 Temp Grad 250 µl
 1H Lineshape 250 µl
 13C S/N ASTM doped 250 µl
 ID 1 250 µl
 ID 2 250 µl
 Sucrose, NMR tested 250 µl

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

Section 2. Hazards identification

OSHA/HCS status	: 1H S/N	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
	4Hz 0.1% H2O/D2O	While this material is not considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200), this MSDS contains valuable information critical to the safe handling and proper use of the product. This MSDS should be retained and available for employees and other users of this product.
	Temp Grad	While this material is not considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200), this MSDS contains valuable information critical to the safe handling and proper use of the product. This MSDS should be retained and available for employees and other users of this product.
	1H Lineshape	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
	13C S/N ASTM doped	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
	ID 1	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
	ID 2	This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
	Sucrose, NMR tested	While this material is not considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200), this MSDS contains valuable information critical to the safe handling and proper use of the product. This MSDS should be retained and available for employees and other users of this product.

Classification of the substance or mixture

1H S/N

H302	ACUTE TOXICITY (oral) - Category 4
H315	SKIN CORROSION/IRRITATION - Category 2
H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2A
H351	CARCINOGENICITY - Category 2
H335 and H336	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Respiratory tract irritation and Narcotic effects) - Category 3
H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2

1H Lineshape

H225	FLAMMABLE LIQUIDS - Category 2
H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2A
H351	CARCINOGENICITY - Category 2
H336	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Narcotic effects) - Category 3
H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2

13C S/N ASTM doped

H225	FLAMMABLE LIQUIDS - Category 2
H302	ACUTE TOXICITY (oral) - Category 4
H315	SKIN CORROSION/IRRITATION - Category 2
H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2A

Section 2. Hazards identification

H340	GERM CELL MUTAGENICITY - Category 1B
H350	CARCINOGENICITY - Category 1A
H335 and H336	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Respiratory tract irritation and Narcotic effects) - Category 3
H372	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 1

ID 1

H302	ACUTE TOXICITY (oral) - Category 4
H315	SKIN CORROSION/IRRITATION - Category 2
H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2A
H351	CARCINOGENICITY - Category 2
H335 and H336	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Respiratory tract irritation and Narcotic effects) - Category 3
H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2

ID 2

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

:	1H S/N	Warning
	4Hz 0.1% H2O/D2O	No signal word.
	Temp Grad	No signal word.
	1H Lineshape	Danger
	13C S/N ASTM doped	Danger
	ID 1	Warning
	ID 2	Warning
	Sucrose, NMR tested	No signal word.

Hazard statements

:	1H S/N	H302 - Harmful if swallowed. H319 - Causes serious eye irritation. H315 - Causes skin irritation. H351 - Suspected of causing cancer. H335 - May cause respiratory irritation. H336 - May cause drowsiness and dizziness. H373 - May cause damage to organs through prolonged or repeated exposure.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	H225 - Highly flammable liquid and vapor. H319 - Causes serious eye irritation. H351 - Suspected of causing cancer. H336 - May cause drowsiness and dizziness. H373 - May cause damage to organs through prolonged or repeated exposure.
	13C S/N ASTM doped	H225 - Highly flammable liquid and vapor. H302 - Harmful if swallowed. H319 - Causes serious eye irritation. H315 - Causes skin irritation. H340 - May cause genetic defects. H350 - May cause cancer. H335 - May cause respiratory irritation. H336 - May cause drowsiness and dizziness.

Section 2. Hazards identification

ID 1	<p>H372 - Causes damage to organs through prolonged or repeated exposure. H302 - Harmful if swallowed. H319 - Causes serious eye irritation. H315 - Causes skin irritation. H351 - Suspected of causing cancer. H335 - May cause respiratory irritation. H336 - May cause drowsiness and dizziness. H373 - May cause damage to organs through prolonged or repeated exposure.</p>
ID 2	<p>H227 - Combustible liquid. H320 - Causes eye irritation. H373 - May cause damage to organs through prolonged or repeated exposure.</p>
Sucrose, NMR tested	No known significant effects or critical hazards.
<u>Precautionary statements</u>	
Prevention	<p>: 1H S/N</p> <p>P201 - Obtain special instructions before use. P202 - Do not handle until all safety precautions have been read and understood. P281 - Use personal protective equipment as required. P280 - Wear protective gloves. Wear eye or face protection. P271 - Use only outdoors or in a well-ventilated area. P260 - Do not breathe vapor. P270 - Do not eat, drink or smoke when using this product. P264 - Wash hands thoroughly after handling. Not applicable. Not applicable. P201 - Obtain special instructions before use. P202 - Do not handle until all safety precautions have been read and understood. P281 - Use personal protective equipment as required. P280 - Wear protective gloves. Wear eye or face protection. P210 - Keep away from heat, sparks, open flames and hot surfaces. - No smoking. P241 - Use explosion-proof electrical, ventilating, lighting and all material-handling equipment. P242 - Use only non-sparking tools. P243 - Take precautionary measures against static discharge. P233 - Keep container tightly closed. P271 - Use only outdoors or in a well-ventilated area. P260 - Do not breathe vapor. P264 - Wash hands thoroughly after handling. P201 - Obtain special instructions before use. P202 - Do not handle until all safety precautions have been read and understood. P281 - Use personal protective equipment as required. P280 - Wear protective gloves. Wear eye or face protection. P210 - Keep away from heat, sparks, open flames and hot surfaces. - No smoking.</p>
4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape	
13C S/N ASTM doped	

Section 2. Hazards identification

13C S/N ASTM doped

ID 1

P304 + P340 + P312 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or physician if you feel unwell.

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.

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.

P314 - Get medical attention if you feel unwell.

P308 + P313 - IF exposed or concerned: Get medical attention.

P304 + P340 + P312 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or physician if you feel unwell.

P301 + P312 + P330 - IF SWALLOWED: Call a POISON CENTER or physician if you feel unwell. Rinse mouth.

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.

P302 + P352 + P362-2 - IF ON SKIN: Wash with plenty of soap and water. Take off contaminated clothing.

P332 + P313 - If skin irritation occurs: Get medical attention.

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.

P314 - Get medical attention if you feel unwell.

P308 + P313 - IF exposed or concerned: Get medical attention.

P304 + P340 + P312 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. Call a POISON CENTER or physician if you feel unwell.

P301 + P312 + P330 - IF SWALLOWED: Call a POISON CENTER or physician if you feel unwell. Rinse mouth.

P302 + P352 + P362-2 + P363 - IF ON SKIN: Wash with plenty of soap and water. Take off contaminated clothing. Wash contaminated clothing before reuse.

P332 + P313 - If skin irritation occurs: Get medical attention.

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.

Section 2. Hazards identification

	ID 2	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. Not applicable.
Storage	Sucrose, NMR tested : 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape	P405 - Store locked up. Not applicable. Not applicable. P405 - Store locked up. P403 - Store in a well-ventilated place. P235 - Keep cool.
	13C S/N ASTM doped	P405 - Store locked up. P403 - Store in a well-ventilated place. P235 - Keep cool.
	ID 1 ID 2	P405 - Store locked up. P403 - Store in a well-ventilated place. P235 - Keep cool.
Disposal	Sucrose, NMR tested : 1H S/N	Not applicable. P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
	4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape	Not applicable. Not applicable. P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
	13C S/N ASTM doped	P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
	ID 1	P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
	ID 2	P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.
Supplemental label elements	Sucrose, NMR tested : 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape	Not applicable. None known. None known. None known. Avoid contact with skin and clothing. Wash thoroughly after handling.
	13C S/N ASTM doped	Avoid contact with skin and clothing. Wash thoroughly after handling.
	ID 1 ID 2	None known. None known.
	Sucrose, NMR tested	None known.
2.3 Other hazards		
Hazards not otherwise classified	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape	None known. None known. None known. Defatting to the skin. Prolonged or repeated contact may dry skin and cause irritation.
	13C S/N ASTM doped	Defatting to the skin. Prolonged or repeated contact may dry skin and cause irritation.
	ID 1	None known.

Section 2. Hazards identification

ID 2	None known.
Sucrose, NMR tested	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	:	1H S/N	Mixture
		4Hz 0.1% H2O/D2O	Mixture
		Temp Grad	Mixture
		1H Lineshape	Mixture
		13C S/N ASTM doped	Mixture
		ID 1	Mixture
		ID 2	Mixture
		Sucrose, NMR tested	Mixture

Ingredient name	%	CAS number
1H S/N		
(² H)Chloroform	60 - 100	865-49-6
Ethylbenzene	< 0.1	100-41-4
1H Lineshape		
(² H ₆)Acetone	60 - 100	666-52-4
Trichloromethane	0.1 - 1	67-66-3
13C S/N ASTM doped		
(² H ₆)Benzene	30 - 60	1076-43-3
1,4-Dioxane	30 - 60	123-91-1
ID 1		
(² H)Chloroform	60 - 100	865-49-6
Iodomethane (¹³ C)	0.1 - 1	4227-95-6
Trimethyl phosphite	0.1 - 1	121-45-9
ID 2		
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	:	1H S/N	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.
		4Hz 0.1% H2O/D2O	Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Get medical attention if irritation occurs.

Section 4. First aid measures

Temp Grad	Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Get medical attention if irritation occurs.
1H Lineshape	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.
13C S/N ASTM doped	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.
ID 1	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.
ID 2	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.
Sucrose, NMR tested	Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Get medical attention if irritation occurs.
Inhalation	
: 1H S/N	Remove victim to fresh air and keep at rest in a position comfortable for breathing. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. 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. If necessary, call a poison center or physician. 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. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
4Hz 0.1% H2O/D2O	Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical attention if symptoms occur.
Temp Grad	Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical attention if symptoms occur.
1H Lineshape	Remove victim to fresh air and keep at rest in a position comfortable for breathing. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. If not breathing, if breathing is irregular or if respiratory arrest

Section 4. First aid measures

13C S/N ASTM doped	<p>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. If necessary, call a poison center or physician. 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. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours. Remove victim to fresh air and keep at rest in a position comfortable for breathing. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. 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. If necessary, call a poison center or physician. 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.</p>
ID 1	<p>Remove victim to fresh air and keep at rest in a position comfortable for breathing. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. 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. If necessary, call a poison center or physician. 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. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.</p>
ID 2	<p>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.</p>
Sucrose, NMR tested	<p>Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical</p>

Section 4. First aid measures

Skin contact	: 1H S/N	attention if symptoms occur.
	4Hz 0.1% H2O/D2O	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Continue to rinse for at least 10 minutes. Get medical attention. Wash clothing before reuse. Clean shoes thoroughly before reuse.
	Temp Grad	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur.
	1H Lineshape	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur.
	13C S/N ASTM doped	Wash skin thoroughly with soap and water or use recognized skin cleanser. Remove contaminated clothing and shoes. Continue to rinse for at least 10 minutes. Get medical attention. Wash clothing before reuse. Clean shoes thoroughly before reuse.
	ID 1	Wash skin thoroughly with soap and water or use recognized skin cleanser. Remove contaminated clothing and shoes. Wash contaminated clothing thoroughly with water before removing it, or wear gloves. Continue to rinse for at least 10 minutes. Get medical attention. Wash clothing before reuse. Clean shoes thoroughly before reuse.
	ID 2	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.
	Sucrose, NMR tested	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur.
Ingestion	: 1H S/N	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. If necessary, call a poison center or physician. 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.
	4Hz 0.1% H2O/D2O	Wash out mouth with water. 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. Do not induce vomiting

Section 4. First aid measures

Temp Grad	<p>unless directed to do so by medical personnel. Get medical attention if symptoms occur.</p> <p>Wash out mouth with water. 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. Do not induce vomiting unless directed to do so by medical personnel. Get medical attention if symptoms occur.</p>
1H Lineshape	<p>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. If necessary, call a poison center or physician. 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.</p>
13C S/N ASTM doped	<p>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. If necessary, call a poison center or physician. 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.</p>
ID 1	<p>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. If necessary, call a poison center or physician. 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.</p>
ID 2	<p>Wash out mouth with water. Remove dentures if any. Remove victim to fresh air and keep at rest in</p>

Section 4. First aid measures

Sucrose, NMR tested

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.

Wash out mouth with water. 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. Do not induce vomiting unless directed to do so by medical personnel. Get medical attention if symptoms occur.

4.2 Most important symptoms/effects, acute and delayed

Potential acute health effects

Eye contact

: 1H S/N
4Hz 0.1% H₂O/D₂O
Temp Grad
1H Lineshape
13C S/N ASTM doped
ID 1
ID 2
Sucrose, NMR tested

Causes serious eye irritation.
No known significant effects or critical hazards.
No known significant effects or critical hazards.
Causes serious eye irritation.
Causes serious eye irritation.
Causes serious eye irritation.
Causes eye irritation.
No known significant effects or critical hazards.

Inhalation

: 1H S/N

4Hz 0.1% H₂O/D₂O
Temp Grad
1H Lineshape

13C S/N ASTM doped

ID 1

ID 2
Sucrose, NMR tested

Can cause central nervous system (CNS) depression. May cause drowsiness and dizziness. May cause respiratory irritation. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure. No known significant effects or critical hazards. No known significant effects or critical hazards. Can cause central nervous system (CNS) depression. May cause drowsiness and dizziness. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure. Can cause central nervous system (CNS) depression. May cause drowsiness and dizziness. May cause respiratory irritation. Can cause central nervous system (CNS) depression. May cause drowsiness and dizziness. May cause respiratory irritation. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure. No known significant effects or critical hazards. No known significant effects or critical hazards.

Section 4. First aid measures

Skin contact	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	Causes skin irritation. No known significant effects or critical hazards. No known significant effects or critical hazards. Defatting to the skin. May cause skin dryness and irritation.			
		31C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Causes skin irritation. Defatting to the skin. Causes skin irritation. No known significant effects or critical hazards. No known significant effects or critical hazards.		
		Ingestion	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	Harmful if swallowed. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach. No known significant effects or critical hazards. No known significant effects or critical hazards. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach.	
				31C S/N ASTM doped	Harmful if swallowed. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach. Harmful if swallowed. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach.
				ID 1	Harmful if swallowed. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach.
	ID 2 Sucrose, NMR tested	May be irritating to mouth, throat and stomach. No known significant effects or critical hazards.			
<u>Over-exposure signs/symptoms</u>					
Eye contact	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	Adverse symptoms may include the following: pain or irritation watering redness			
		No specific data. No specific data.			
		Adverse symptoms may include the following: pain or irritation watering redness			
		31C S/N ASTM doped	Adverse symptoms may include the following: pain or irritation watering redness		
		ID 1	Adverse symptoms may include the following: pain or irritation watering redness		
	ID 2 Sucrose, NMR tested	Adverse symptoms may include the following: irritation watering redness No specific data.			
Inhalation	: 1H S/N	Adverse symptoms may include the following: respiratory tract irritation coughing nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness			
		4Hz 0.1% H2O/D2O Temp Grad	No specific data. No specific data.		

Section 4. First aid measures

	1H Lineshape	Adverse symptoms may include the following: nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness
	13C S/N ASTM doped	Adverse symptoms may include the following: respiratory tract irritation coughing nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness
	ID 1	Adverse symptoms may include the following: respiratory tract irritation coughing nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness
	ID 2 Sucrose, NMR tested	No specific data. No specific data.
Skin contact	: 1H S/N	Adverse symptoms may include the following: irritation redness
	4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape	No specific data. No specific data. Adverse symptoms may include the following: irritation dryness cracking
	13C S/N ASTM doped	Adverse symptoms may include the following: irritation redness dryness cracking
	ID 1	Adverse symptoms may include the following: irritation redness
	ID 2 Sucrose, NMR tested	No specific data. No specific data.
Ingestion	: 1H S/N	No specific data.
	4Hz 0.1% H ₂ O/D ₂ O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	No specific data.
	13C S/N ASTM doped	No specific data.
	ID 1	No specific data.
	ID 2	No specific data.
	Sucrose, NMR tested	No specific data.

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

Section 4. First aid measures

Notes to physician	: 1H S/N	In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
	4Hz 0.1% H2O/D2O	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
	Temp Grad	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
	1H Lineshape	In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
	13C S/N ASTM doped	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
	ID 1	In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
	ID 2	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
	Sucrose, NMR tested	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
Specific treatments	: 1H S/N	No specific treatment.
	4Hz 0.1% H2O/D2O	No specific treatment.
	Temp Grad	No specific treatment.
	1H Lineshape	No specific treatment.
	13C S/N ASTM doped	No specific treatment.
	ID 1	No specific treatment.
	ID 2	No specific treatment.
	Sucrose, NMR tested	No specific treatment.
Protection of first-aiders	: 1H S/N	No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.
	4Hz 0.1% H2O/D2O	No action shall be taken involving any personal risk or without suitable training.
	Temp Grad	No action shall be taken involving any personal risk or without suitable training.
	1H Lineshape	No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.
	13C S/N ASTM doped	No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Wash contaminated clothing thoroughly with water before removing it, or wear gloves.

Section 4. First aid measures

ID 1	No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.
ID 2	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.
Sucrose, NMR tested	No action shall be taken involving any personal risk or without suitable training.

See toxicological information (Section 11)

Section 5. Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Use an extinguishing agent suitable for the surrounding fire. Use an extinguishing agent suitable for the surrounding fire. Use an extinguishing agent suitable for the surrounding fire. Use dry chemical, CO ₂ , water spray (fog) or foam. Use dry chemical, CO ₂ , water spray (fog) or foam. Use an extinguishing agent suitable for the surrounding fire. Use dry chemical, CO ₂ , water spray (fog) or foam. Use an extinguishing agent suitable for the surrounding fire.
Unsuitable extinguishing media	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	None known. None known. None known. Do not use water jet. Do not use water jet. None known. Do not use water jet. None known.

5.2 Special hazards arising from the substance or mixture

Specific hazards arising from the chemical	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape 13C S/N ASTM doped	In a fire or if heated, a pressure increase will occur and the container may burst. In a fire or if heated, a pressure increase will occur and the container may burst. In a fire or if heated, a pressure increase will occur and the container may burst. Highly flammable liquid and vapor. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. Runoff to sewer may create fire or explosion hazard. Highly flammable liquid and vapor. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. Runoff to sewer may create fire or explosion hazard.
---	---	---

Section 5. Fire-fighting measures

	ID 1	In a fire or if heated, a pressure increase will occur and the container may burst.
	ID 2	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.
	Sucrose, NMR tested	In a fire or if heated, a pressure increase will occur and the container may burst.
Hazardous thermal decomposition products	: Decomposition products may include the following materials: carbon dioxide carbon monoxide sulfur oxides halogenated compounds carbonyl halides	
5.3 Advice for firefighters		
Special protective actions for fire-fighters	: 1H S/N	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.
	4Hz 0.1% H2O/D2O	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.
	Temp Grad	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.
	1H Lineshape	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.
	13C S/N ASTM doped	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.
	ID 1	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.
	ID 2	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.
	Sucrose, NMR tested	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.

Section 5. Fire-fighting measures

Special protective equipment for fire-fighters	: 1H S/N	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
	4Hz 0.1% H ₂ O/D ₂ O	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
	Temp Grad	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
	1H Lineshape	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
	13C S/N ASTM doped	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
	ID 1	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
	ID 2	Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.
	Sucrose, NMR tested	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. Do not breathe 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

- : 1H S/N
- 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).
- 4Hz 0.1% H₂O/D₂O
- 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).
- Temp Grad
- Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

Section 6. Accidental release measures

	Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).
1H Lineshape	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).
13C S/N ASTM doped	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).
ID 1	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).
ID 2	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).
Sucrose, NMR tested	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

1H S/N	Stop leak if without risk. Move containers from spill area. 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.
4Hz 0.1% H ₂ O/D ₂ O	Stop leak if without risk. Move containers from spill area. 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.
Temp Grad	Stop leak if without risk. Move containers from spill area. 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.
1H Lineshape	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.
13C S/N ASTM doped	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.
ID 1	Stop leak if without risk. Move containers from spill area. 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.
ID 2	Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Dilute with water and mop

Section 6. Accidental release measures

Sucrose, NMR tested

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.
Stop leak if without risk. Move containers from spill area. 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 : 1H S/N

4Hz 0.1% H₂O/D₂O

Temp Grad

1H Lineshape

13C S/N ASTM doped

Put on appropriate personal protective equipment (see Section 8). Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Do not get in eyes or on skin or clothing. Do not breathe vapor or mist. Do not ingest. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Empty containers retain product residue and can be hazardous. Do not reuse container.

Put on appropriate personal protective equipment (see Section 8).

Put on appropriate personal protective equipment (see Section 8).

Put on appropriate personal protective equipment (see Section 8). Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Do not get in eyes or on skin or clothing. Do not breathe vapor or mist. Do not ingest. 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. Take precautionary measures against electrostatic discharges. Empty containers retain product residue and can be hazardous. Do not reuse container.

Put on appropriate personal protective equipment (see Section 8). Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Do not get in eyes or on skin or clothing. Do not breathe vapor or mist. Do not ingest. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated.

Section 7. Handling and storage

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. Take precautionary measures against electrostatic discharges. Empty containers retain product residue and can be hazardous. Do not reuse container.

ID 1

Put on appropriate personal protective equipment (see Section 8). Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Do not get in eyes or on skin or clothing. Do not breathe vapor or mist. Do not ingest. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Empty containers retain product residue and can be hazardous. Do not reuse container.

ID 2

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.

Sucrose, NMR tested

Put on appropriate personal protective equipment (see Section 8).

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

: 1H S/N

Store in accordance with local regulations. 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. Store locked up. 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

Section 7. Handling and storage

4Hz 0.1% H₂O/D₂O

environmental contamination.

Store in accordance with local regulations. 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. 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.

Temp Grad

Store in accordance with local regulations. 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. 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.

1H Lineshape

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. Store locked up. 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.

13C S/N ASTM doped

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. Store locked up. 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.

ID 1

Store in accordance with local regulations. 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. Store locked up. 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

Section 7. Handling and storage

ID 2

environmental contamination.
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.

Sucrose, NMR tested

Store in accordance with local regulations. 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. 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.

7.3 Specific end use(s)

Recommendations

: 1H S/N	Industrial applications, Professional applications.
4Hz 0.1% H ₂ O/D ₂ O	Industrial applications, Professional applications.
Temp Grad	Industrial applications, Professional applications.
1H Lineshape	Industrial applications, Professional applications.
13C S/N ASTM doped	Industrial applications, Professional applications.
ID 1	Industrial applications, Professional applications.
ID 2	Industrial applications, Professional applications.
Sucrose, NMR tested	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
1H S/N (² H)Chloroform	<p>ACGIH TLV (United States, 3/2012). TWA: 10 ppm 8 hours. TWA: 49 mg/m³ 8 hours.</p> <p>OSHA PEL 1989 (United States, 3/1989). TWA: 2 ppm 8 hours. TWA: 9.78 mg/m³ 8 hours.</p> <p>NIOSH REL (United States, 6/2009). STEL: 2 ppm 60 minutes. STEL: 9.78 mg/m³ 60 minutes.</p> <p>OSHA PEL (United States, 6/2010).</p>

Section 8. Exposure controls/personal protection

Ethylbenzene

CEIL: 50 ppm
 CEIL: 240 mg/m³
ACGIH TLV (United States, 6/2013).
 TWA: 20 ppm 8 hours.
NIOSH REL (United States, 4/2013).
 STEL: 545 mg/m³ 15 minutes.
 STEL: 125 ppm 15 minutes.
 TWA: 435 mg/m³ 10 hours.
 TWA: 100 ppm 10 hours.
OSHA PEL (United States, 2/2013).
 TWA: 435 mg/m³ 8 hours.
 TWA: 100 ppm 8 hours.
OSHA PEL 1989 (United States, 3/1989).
 STEL: 545 mg/m³ 15 minutes.
 STEL: 125 ppm 15 minutes.
 TWA: 435 mg/m³ 8 hours.
 TWA: 100 ppm 8 hours.

1H Lineshape
 (²H₆)Acetone

ACGIH TLV (United States, 3/2012).
 TWA: 500 ppm 8 hours.
 TWA: 1188 mg/m³ 8 hours.
 STEL: 750 ppm 15 minutes.
 STEL: 1782 mg/m³ 15 minutes.
OSHA PEL 1989 (United States, 3/1989).
 TWA: 750 ppm 8 hours.
 TWA: 1800 mg/m³ 8 hours.
 STEL: 1000 ppm 15 minutes.
 STEL: 2400 mg/m³ 15 minutes.
NIOSH REL (United States, 6/2009).
 TWA: 250 ppm 10 hours.
 TWA: 590 mg/m³ 10 hours.
OSHA PEL (United States, 6/2010).
 TWA: 1000 ppm 8 hours.
 TWA: 2400 mg/m³ 8 hours.

Trichloromethane

ACGIH TLV (United States, 6/2013).
 TWA: 49 mg/m³ 8 hours.
 TWA: 10 ppm 8 hours.
NIOSH REL (United States, 4/2013).
 STEL: 9.78 mg/m³ 60 minutes.
 STEL: 2 ppm 60 minutes.
OSHA PEL (United States, 2/2013).
 CEIL: 240 mg/m³
 CEIL: 50 ppm
OSHA PEL 1989 (United States, 3/1989).
 TWA: 9.78 mg/m³ 8 hours.
 TWA: 2 ppm 8 hours.

13C S/N ASTM doped
 (²H₆)Benzene

ACGIH TLV (United States, 3/2012).
Absorbed through skin.
 TWA: 0.5 ppm 8 hours.
 TWA: 1.6 mg/m³ 8 hours.
 STEL: 2.5 ppm 15 minutes.
 STEL: 8 mg/m³ 15 minutes.
OSHA PEL 1989 (United States, 3/1989).
 TWA: 1 ppm 8 hours.

Section 8. Exposure controls/personal protection

1,4-Dioxane

STEL: 5 ppm 15 minutes.
OSHA PEL Z2 (United States, 11/2006).
 TWA: 10 ppm 8 hours.
 CEIL: 25 ppm
 AMP: 50 ppm 10 minutes.
NIOSH REL (United States, 6/2009).
 TWA: 0.1 ppm 10 hours.
 STEL: 1 ppm 15 minutes.
OSHA PEL (United States, 6/2010).
 TWA: 1 ppm 8 hours.
 STEL: 5 ppm 15 minutes.
OSHA PEL 1989 (United States, 3/1989).
Absorbed through skin.
 TWA: 25 ppm 8 hours.
 TWA: 90 mg/m³ 8 hours.
NIOSH REL (United States, 4/2013).
 CEIL: 1 ppm 30 minutes.
 CEIL: 3.6 mg/m³ 30 minutes.
ACGIH TLV (United States, 6/2013).
Absorbed through skin.
 TWA: 20 ppm 8 hours.
OSHA PEL (United States, 2/2013).
Absorbed through skin.
 TWA: 100 ppm 8 hours.
 TWA: 360 mg/m³ 8 hours.

ID 1
 (²H)Chloroform

ACGIH TLV (United States, 3/2012).
 TWA: 10 ppm 8 hours.
 TWA: 49 mg/m³ 8 hours.
OSHA PEL 1989 (United States, 3/1989).
 TWA: 2 ppm 8 hours.
 TWA: 9.78 mg/m³ 8 hours.
NIOSH REL (United States, 6/2009).
 STEL: 2 ppm 60 minutes.
 STEL: 9.78 mg/m³ 60 minutes.
OSHA PEL (United States, 6/2010).
 CEIL: 50 ppm
 CEIL: 240 mg/m³

Iodomethane (¹³ C)

ACGIH TLV (United States, 3/2012).
Absorbed through skin.
 TWA: 2 ppm 8 hours.
OSHA PEL 1989 (United States, 3/1989).
Absorbed through skin.
 TWA: 2 ppm 8 hours.
 TWA: 10 mg/m³ 8 hours.
NIOSH REL (United States, 6/2009).
Absorbed through skin.
 TWA: 2 ppm 10 hours.
 TWA: 10 mg/m³ 10 hours.
OSHA PEL (United States, 6/2010).
Absorbed through skin.
 TWA: 5 ppm 8 hours.
 TWA: 28 mg/m³ 8 hours.

Trimethyl phosphite

ACGIH TLV (United States, 6/2013).
 TWA: 2 ppm 8 hours.
 TWA: 10 mg/m³ 8 hours.

Section 8. Exposure controls/personal protection

ID 2

di[(²H₃)Methyl] sulphoxide

OSHA PEL 1989 (United States, 3/1989).

TWA: 2 ppm 8 hours.

TWA: 10 mg/m³ 8 hours.

NIOSH REL (United States, 4/2013).

TWA: 2 ppm 10 hours.

TWA: 10 mg/m³ 10 hours.

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. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves.

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.

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	: 1H S/N	Liquid.
	4Hz 0.1% H2O/D2O	Liquid.
	Temp Grad	Liquid.
	1H Lineshape	Liquid.
	13C S/N ASTM doped	Liquid.
	ID 1	Liquid.
	ID 2	Liquid. [Clear.]
Color	Sucrose, NMR tested	Liquid. [Clear.]
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Colorless.
	Temp Grad	Colorless.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
Odor	ID 2	Colorless.
	Sucrose, NMR tested	Not available.
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
Odor threshold	ID 1	Not available.
	ID 2	Ripe olive.
	Sucrose, NMR tested	Not available.
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
pH	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	7
	Temp Grad	Not available.
Melting point	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
	: 1H S/N	-64°C (-83.2°F)
	4Hz 0.1% H2O/D2O	3.81°C (38.9°F)
Temp Grad	3.81°C (38.9°F)	
1H Lineshape	-95°C (-139°F)	
13C S/N ASTM doped	Not available.	
ID 1	-64°C (-83.2°F)	
ID 2	18 to 18.54°C (64.4 to 65.4°F)	
Sucrose, NMR tested	0°C (32°F)	

Section 9. Physical and chemical properties

Boiling point	: 1H S/N	60.9°C (141.6°F)
	4Hz 0.1% H ₂ O/D ₂ O	101.42°C (214.6°F)
	Temp Grad	101.42°C (214.6°F)
	1H Lineshape	55.5°C (131.9°F)
	13C S/N ASTM doped	90°C (194°F)
	ID 1	60.9°C (141.6°F)
	ID 2	189°C (372.2°F)
	Sucrose, NMR tested	100°C (212°F)
Flash point	: 1H S/N	Not available.
	4Hz 0.1% H ₂ O/D ₂ O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Closed cup: -17°C (1.4°F)
	13C S/N ASTM doped	Closed cup: 21.1°C (70°F)
	ID 1	Not available.
	ID 2	Closed cup: 88°C (190.4°F)
	Sucrose, NMR tested	Not available.
Evaporation rate	: 1H S/N	Not available.
	4Hz 0.1% H ₂ O/D ₂ O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
Flammability (solid, gas)	: 1H S/N	Not available.
	4Hz 0.1% H ₂ O/D ₂ O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
Lower and upper explosive (flammable) limits	: 1H S/N	Not available.
	4Hz 0.1% H ₂ O/D ₂ O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Lower: 3%
	Sucrose, NMR tested	Not available.
Vapor pressure	: 1H S/N	Not available.
	4Hz 0.1% H ₂ O/D ₂ O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	0.061 kPa (0.46 mm Hg) [room temperature]
	Sucrose, NMR tested	Not available.
Vapor density	: 1H S/N	Not available.
	4Hz 0.1% H ₂ O/D ₂ O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	1.04 [Air = 1]
	Sucrose, NMR tested	Not available.

Section 9. Physical and chemical properties

Relative density	: 1H S/N	1.5
	4Hz 0.1% H2O/D2O	1.1
	Temp Grad	1.1
	1H Lineshape	0.872
	13C S/N ASTM doped	0.98
	ID 1	1500
	ID 2	1.18
	Sucrose, NMR tested	Not available.
Solubility	: 1H S/N	Very slightly soluble in the following materials: cold water and hot water.
	4Hz 0.1% H2O/D2O	Easily soluble in the following materials: cold water and hot water.
	Temp Grad	Easily soluble in the following materials: cold water and hot water.
	1H Lineshape	Easily soluble in the following materials: cold water, hot water and acetone.
	13C S/N ASTM doped	Easily soluble in the following materials: cold water and hot water.
	ID 1	Very slightly soluble in the following materials: cold water and hot water.
	ID 2	Soluble in the following materials: cold water and hot water.
	Sucrose, NMR tested	Easily soluble in the following materials: cold water and hot water.
Solubility in water	: Not available.	
Partition coefficient: n-octanol/water	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
Auto-ignition temperature	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	215°C (419°F)
	Sucrose, NMR tested	Not available.
Decomposition temperature	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
Viscosity	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.

Section 10. Stability and reactivity

10.1 Reactivity	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	No specific test data related to reactivity available for this product or its ingredients. No specific test data related to reactivity available for this product or its ingredients. No specific test data related to reactivity available for this product or its ingredients. No specific test data related to reactivity available for this product or its ingredients. No specific test data related to reactivity available for this product or its ingredients. No specific test data related to reactivity available for this product or its ingredients. No specific test data related to reactivity available for this product or its ingredients. No specific test data related to reactivity available for this product or its ingredients.
10.2 Chemical stability	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	The product is stable. The product is stable. The product is stable. The product is stable. The product is stable. The product is stable. The product is stable. The product is stable.
10.3 Possibility of hazardous reactions	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Under normal conditions of storage and use, hazardous reactions will not occur. Under normal conditions of storage and use, hazardous reactions will not occur. Under normal conditions of storage and use, hazardous reactions will not occur. Under normal conditions of storage and use, hazardous reactions will not occur. Under normal conditions of storage and use, hazardous reactions will not occur. Under normal conditions of storage and use, hazardous reactions will not occur. Under normal conditions of storage and use, hazardous reactions will not occur. Under normal conditions of storage and use, hazardous reactions will not occur.
10.4 Conditions to avoid	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2	No specific data. No specific data. No specific data. 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. 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. No specific data. Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder,

Section 10. Stability and reactivity

	Sucrose, NMR tested	drill, grind or expose containers to heat or sources of ignition. Do not allow vapor to accumulate in low or confined areas. No specific data.
10.5 Incompatible materials	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	No specific data. No specific data. No specific data. Reactive or incompatible with the following materials: oxidizing materials
	13C S/N ASTM doped	Reactive or incompatible with the following materials: oxidizing materials
	ID 1 ID 2	No specific data. Reactive or incompatible with the following materials: oxidizing materials
	Sucrose, NMR tested	No specific data.
10.6 Hazardous decomposition products	: 1H S/N	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
	4Hz 0.1% H2O/D2O	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
	Temp Grad	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
	1H Lineshape	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
	13C S/N ASTM doped	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
	ID 1	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
	ID 2	Under normal conditions of storage and use, hazardous decomposition products should not be produced.
	Sucrose, NMR tested	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

Section 11. Toxicological information

Product/ingredient name	Result	Species	Dose	Exposure
1H S/N (² H)Chloroform	LC50 Inhalation Vapor LD50 Dermal	Rat Rabbit	47702 mg/m ³ >20 g/kg	4 hours -
Ethylbenzene	LD50 Oral LC50 Inhalation Gas. LD50 Dermal LD50 Oral	Rat Rabbit Rat	300 mg/kg 4000 ppm >5000 mg/kg 3500 mg/kg	- 4 hours - -
1H Lineshape (² H ₆)Acetone Trichloromethane	LD50 Oral LC50 Inhalation Vapor LD50 Dermal LD50 Oral	Rat Rat Rabbit Rat	5800 mg/kg 47702 mg/m ³ >20 g/kg 300 mg/kg	- 4 hours - -
13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	LD50 Oral LD50 Oral	Rat Rat	930 mg/kg 4200 mg/kg	- -
ID 1 (² H)Chloroform	LC50 Inhalation Vapor LD50 Dermal LD50 Oral	Rat Rabbit Rat	47702 mg/m ³ >20 g/kg 300 mg/kg	4 hours - -
Iodomethane (¹³ C)	LC50 Inhalation Vapor LD50 Oral	Rat Rat	1300 mg/m ³ 76 mg/kg	4 hours -
Trimethyl phosphite	LC50 Inhalation Vapor LD50 Dermal LD50 Oral	Rat Rabbit Rat	182000 mg/m ³ 933.8 mg/kg 1350 mg/kg	1 hours - -
ID 2 di[(² H ₃)Methyl] sulphoxide	LD50 Dermal LD50 Oral	Rat Rat	40000 mg/kg 14500 mg/kg	- -

Irritation/Corrosion

Product/ingredient name	Result	Species	Score	Exposure	Observation
1H S/N (² H)Chloroform	Eyes - Moderate irritant Skin - Mild irritant	Rabbit Rabbit	- -	24 hours 20 milligrams 24 hours 500 milligrams	- -
Ethylbenzene	Skin - Mild irritant	Rabbit	-	24 hours 15 milligrams	-
1H Lineshape (² H ₆)Acetone	Eyes - Mild irritant Eyes - Mild irritant Eyes - Moderate irritant Eyes - Severe irritant Skin - Mild irritant Skin - Mild irritant	Human Rabbit Rabbit Rabbit Rabbit Rabbit	- - - - - -	186300 parts per million 10 microliters 24 hours 20 milligrams 20 milligrams 24 hours 500 milligrams 395 milligrams	- - - - - -
Trichloromethane	Eyes - Moderate irritant Skin - Mild irritant	Rabbit Rabbit	- -	24 hours 20 milligrams 24 hours 500 milligrams	- -

Section 11. Toxicological information

13C S/N ASTM doped (² H ₆)Benzene	Eyes - Moderate irritant	Rabbit	-	milligrams	-
	Eyes - Severe irritant	Rabbit	-	88 milligrams	-
	Skin - Mild irritant	Rat	-	24 hours 2	-
				milligrams	-
	Skin - Mild irritant	Rabbit	-	8 hours 60	-
				microliters	-
1,4-Dioxane	Skin - Moderate irritant	Rabbit	-	24 hours 15	-
				milligrams	-
	Eyes - Moderate irritant	Rabbit	-	24 hours 20	-
				milligrams	-
Skin - Mild irritant	Rabbit	-	24 hours 100	-	
			milligrams	-	
ID 1 (² H)Chloroform	Eyes - Moderate irritant	Rabbit	-	515	-
	milligrams	-	-	-	
Iodomethane (¹³ C)	Skin - Mild irritant	Rabbit	-	24 hours 20	-
				milligrams	-
	Eyes - Severe irritant	Rabbit	-	24 hours 500	-
				milligrams	-
Trimethyl phosphite	Skin - Mild irritant	Human	-	100	-
				milligrams	-
				30 minutes 1	-
ID 2 di[(² H ₃)Methyl] sulphoxide	Skin - Severe irritant	Rabbit	-	Grams	-
				500	-
	Eyes - Mild irritant	Rabbit	-	milligrams	-
				10 minutes 1	-
Eyes - Mild irritant	Rabbit	-	Grams	-	
			0.1 Milliliters	-	
di[(² H ₃)Methyl] sulphoxide	Skin - Severe irritant	Rabbit	-	500	-
				milligrams	-
	Eyes - Mild irritant	Rabbit	-	500	-
				milligrams	-
Skin - Mild irritant	Rabbit	-	100	-	
			milligrams	-	
Skin - Mild irritant	Rabbit	-	100	-	
			milligrams	-	

Sensitization

Not available.

Mutagenicity

Not available.

Carcinogenicity

Not available.

Classification

Section 11. Toxicological information

Product/ingredient name	OSHA	IARC	NTP
1H S/N (² H)Chloroform Ethylbenzene	- -	2B 2B	Reasonably anticipated to be a human carcinogen. -
1H Lineshape Trichloromethane	-	2B	Reasonably anticipated to be a human carcinogen.
13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	+ -	1 2B	Known to be a human carcinogen. Reasonably anticipated to be a human carcinogen.
ID 1 (² H)Chloroform Iodomethane (¹³ C)	- -	2B 3	Reasonably anticipated to be a human carcinogen. -

Reproductive toxicity

Not available.

Teratogenicity

Not available.

Specific target organ toxicity (single exposure)

Name	Category	Route of exposure	Target organs
1H S/N (² H)Chloroform	Category 3	Not applicable.	Respiratory tract irritation and Narcotic effects
Ethylbenzene	Category 3	Not applicable.	Respiratory tract irritation and Narcotic effects
1H Lineshape (² H ₆)Acetone Trichloromethane	Category 3 Category 3	Not applicable. Not applicable.	Narcotic effects Respiratory tract irritation and Narcotic effects
13C S/N ASTM doped (² H ₆)Benzene	Category 3	Not applicable.	Respiratory tract irritation and Narcotic effects
1,4-Dioxane	Category 3	Not applicable.	Respiratory tract irritation
ID 1 (² H)Chloroform	Category 3	Not applicable.	Respiratory tract irritation and Narcotic effects
Iodomethane (¹³ C)	Category 3	Not applicable.	Respiratory tract irritation
Trimethyl phosphite	Category 3	Not applicable.	Respiratory tract irritation

Specific target organ toxicity (repeated exposure)

Section 11. Toxicological information

Name	Category	Route of exposure	Target organs
1H S/N (² H)Chloroform	Category 2	Not determined	kidneys and liver
1H Lineshape Trichloromethane	Category 2	Not determined	heart, kidneys and liver
13C S/N ASTM doped (² H ₆)Benzene	Category 1	Oral	blood system
1,4-Dioxane	Category 1	Inhalation Oral	blood system kidneys and liver
ID 1 (² H)Chloroform	Category 2	Not determined	kidneys and liver
ID 2 di[(² H ₃)Methyl] sulphoxide	Category 2	Oral	kidneys and liver

Aspiration hazard

Name	Result
1H S/N (² H)Chloroform Ethylbenzene	ASPIRATION HAZARD - Category 1 ASPIRATION HAZARD - Category 1
13C S/N ASTM doped (² H ₆)Benzene	ASPIRATION HAZARD - Category 1
ID 1 (² H)Chloroform	ASPIRATION HAZARD - Category 1

Information on the likely routes of exposure : Not available.

Potential acute health effects

Eye contact	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Causes serious eye irritation. No known significant effects or critical hazards. No known significant effects or critical hazards. Causes serious eye irritation. Causes serious eye irritation. Causes serious eye irritation. Causes eye irritation. No known significant effects or critical hazards.
Inhalation	: 1H S/N 4Hz 0.1% H ₂ O/D ₂ O Temp Grad 1H Lineshape	Can cause central nervous system (CNS) depression. May cause drowsiness and dizziness. May cause respiratory irritation. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure. No known significant effects or critical hazards. No known significant effects or critical hazards. Can cause central nervous system (CNS) depression. May cause drowsiness and dizziness. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure.

Section 11. Toxicological information

	13C S/N ASTM doped	Can cause central nervous system (CNS) depression. May cause drowsiness and dizziness. May cause respiratory irritation.
	ID 1	Can cause central nervous system (CNS) depression. May cause drowsiness and dizziness. May cause respiratory irritation. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure.
	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.
Skin contact	: 1H S/N	Causes skin irritation.
	4Hz 0.1% H ₂ O/D ₂ O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Defatting to the skin. May cause skin dryness and irritation.
	13C S/N ASTM doped	Causes skin irritation. Defatting to the skin.
	ID 1	Causes skin irritation.
	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.
Ingestion	: 1H S/N	Harmful if swallowed. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach.
	4Hz 0.1% H ₂ O/D ₂ O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach.
	13C S/N ASTM doped	Harmful if swallowed. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach.
	ID 1	Harmful if swallowed. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach.
	ID 2	May be irritating to mouth, throat and stomach.
	Sucrose, NMR tested	No known significant effects or critical hazards.

Symptoms related to the physical, chemical and toxicological characteristics

Eye contact	: 1H S/N	Adverse symptoms may include the following: pain or irritation watering redness
	4Hz 0.1% H ₂ O/D ₂ O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	Adverse symptoms may include the following: pain or irritation watering redness
	13C S/N ASTM doped	Adverse symptoms may include the following: pain or irritation watering redness
	ID 1	Adverse symptoms may include the following: pain or irritation watering redness
	ID 2	Adverse symptoms may include the following: irritation watering redness

Section 11. Toxicological information

	Sucrose, NMR tested	No specific data.
Inhalation	: 1H S/N	Adverse symptoms may include the following: respiratory tract irritation coughing nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness
	4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	No specific data. No specific data. Adverse symptoms may include the following: nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness
	13C S/N ASTM doped	Adverse symptoms may include the following: respiratory tract irritation coughing nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness
	ID 1	Adverse symptoms may include the following: respiratory tract irritation coughing nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness
	ID 2 Sucrose, NMR tested	No specific data. No specific data.
Skin contact	: 1H S/N	Adverse symptoms may include the following: irritation redness
	4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	No specific data. No specific data. Adverse symptoms may include the following: irritation dryness cracking
	13C S/N ASTM doped	Adverse symptoms may include the following: irritation redness dryness cracking
	ID 1	Adverse symptoms may include the following: irritation redness
	ID 2 Sucrose, NMR tested	No specific data. No specific data.

Section 11. Toxicological information

Ingestion	: 1H S/N	No specific data.
	4Hz 0.1% H2O/D2O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	No specific data.
	13C S/N ASTM doped	No specific data.
	ID 1	No specific data.
	ID 2	No specific data.
	Sucrose, NMR tested	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	: 1H S/N	May cause damage to organs through prolonged or repeated exposure.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	May cause damage to organs through prolonged or repeated exposure. Prolonged or repeated contact can defat the skin and lead to irritation, cracking and/or dermatitis.
	13C S/N ASTM doped	Causes damage to organs through prolonged or repeated exposure. Prolonged or repeated contact can defat the skin and lead to irritation, cracking and/or dermatitis.
	ID 1	May cause damage to organs through prolonged or repeated exposure.
	ID 2	May cause damage to organs through prolonged or repeated exposure.
	Sucrose, NMR tested	No known significant effects or critical hazards.
Carcinogenicity	: 1H S/N	Suspected of causing cancer. Risk of cancer depends on duration and level of exposure.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Suspected of causing cancer. Risk of cancer depends on duration and level of exposure.
	13C S/N ASTM doped	May cause cancer. Risk of cancer depends on duration and level of exposure.
	ID 1	Suspected of causing cancer. Risk of cancer depends on duration and level of exposure.
	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.

Section 11. Toxicological information

Mutagenicity	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. May cause genetic defects. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards.
Teratogenicity	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards.
Developmental effects	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards.
Fertility effects	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards. No known significant effects or critical hazards.

Numerical measures of toxicity

Acute toxicity estimates

Route	ATE value
1H S/N Oral	500.5 mg/kg
1H Lineshape Oral	30000 mg/kg
13C S/N ASTM doped Oral	1360.7 mg/kg
ID 1 Oral Dermal Inhalation (vapors)	477.3 mg/kg 50505.5 mg/kg 300 mg/l
ID 2 Oral	25000 mg/kg

Section 11. Toxicological information

Other information	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.

Section 12. Ecological information

12.1 Toxicity

Product/ingredient name	Result	Species	Exposure	
1H S/N (² H)Chloroform	Acute EC50 13.3 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours	
	Acute LC50 81.5 mg/l Marine water	Crustaceans - Penaeus duorarum	48 hours	
	Acute LC50 29000 µg/l Fresh water	Daphnia - Daphnia magna	48 hours	
	Acute LC50 13300 µg/l Fresh water	Fish - Lepomis macrochirus	96 hours	
	Chronic EC10 3.61 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours	
	Ethylbenzene	Chronic NOEC 6300 µg/l Fresh water	Daphnia - Daphnia magna	21 days
		Acute EC50 4600 µg/l Fresh water	Algae - Pseudokirchneriella subcapitata	72 hours
Acute EC50 3600 µg/l Fresh water		Algae - Pseudokirchneriella subcapitata	96 hours	
Acute EC50 2970 µg/l Fresh water		Daphnia - Daphnia magna - Neonate	48 hours	
Acute LC50 5200 µg/l Marine water		Crustaceans - Americamysis bahia	48 hours	
Acute LC50 4200 µg/l Fresh water		Fish - Oncorhynchus mykiss	96 hours	
Chronic NOEC 1000 µg/l Fresh water		Algae - Pseudokirchneriella subcapitata	96 hours	
1H Lineshape (² H ₆)Acetone	Acute EC50 20.565 mg/l Marine water	Algae - Ulva pertusa	96 hours	
	Acute LC50 6000000 µg/l Fresh water	Crustaceans - Gammarus pulex	48 hours	
	Acute LC50 10000 µg/l Fresh water	Daphnia - Daphnia magna	48 hours	
	Acute LC50 100000 µg/l Fresh water	Fish - Pimephales promelas - Juvenile (Fledgling, Hatchling, Weanling)	96 hours	
	Chronic NOEC 4.95 mg/l Marine water	Algae - Ulva pertusa	96 hours	
Trichloromethane	Chronic NOEC 0.1 ml/L Fresh water	Daphnia - Daphnia magna - Neonate	21 days	
	Acute EC50 13.3 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours	
	Acute EC50 2.803 mg/l Fresh water	Crustaceans - Cypris subglobosa	48 hours	
	Acute LC50 63800 µg/l Fresh water	Daphnia - Daphnia magna - Neonate	48 hours	
	Acute LC50 13.3 ppm Fresh water	Fish - Lepomis macrochirus	96 hours	
	Chronic EC10 3.61 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours	
	Chronic NOEC 6300 µg/l Fresh water	Daphnia - Daphnia magna	21 days	

Section 12. Ecological information

13C S/N ASTM doped (² H ₆)Benzene	Acute EC50 29000 µg/l Fresh water	Algae - Pseudokirchneriella subcapitata	72 hours
	Acute EC50 1360000 µg/l Fresh water	Algae - Scenedesmus abundans	96 hours
	Acute EC50 9230 µg/l Fresh water	Daphnia - Daphnia magna - Neonate	48 hours
	Acute LC50 21000 µg/l Marine water	Crustaceans - Artemia salina - Nauplii	48 hours
	Acute LC50 5.28 ul/L Fresh water	Fish - Oncorhynchus gorbuscha - Fry	96 hours
	Chronic NOEC 1.5 to 5.4 ul/L Marine water	Fish - Morone saxatilis - Juvenile (Fledgling, Hatchling, Weanling)	4 weeks
1,4-Dioxane	Acute LC50 6700000 µg/l Marine water	Fish - Menidia beryllina	96 hours
ID 1 (² H)Chloroform	Acute EC50 13.3 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours
	Acute LC50 81.5 mg/l Marine water	Crustaceans - Penaeus duorarum	48 hours
	Acute LC50 29000 µg/l Fresh water	Daphnia - Daphnia magna	48 hours
	Acute LC50 13300 µg/l Fresh water	Fish - Lepomis macrochirus	96 hours
	Chronic EC10 3.61 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours
ID 2 di[(² H ₃)Methyl] sulphoxide	Chronic NOEC 6300 µg/l Fresh water	Daphnia - Daphnia magna	21 days
	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

Product/ingredient name	Aquatic half-life	Photolysis	Biodegradability
1H S/N Ethylbenzene	-	-	Readily

12.3 Bioaccumulative potential

Product/ingredient name	LogP _{ow}	BCF	Potential
1H S/N (² H)Chloroform Ethylbenzene	1.97	690	high
	3.6	-	low
1H Lineshape (² H ₆)Acetone Trichloromethane	-0.23	-	low
	1.97	690	high
13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	2.13	11	low
	-0.42	0.3 to 0.7	low
ID 1 (² H)Chloroform Iodomethane (¹³ C) Trimethyl phosphite	1.97	690	high
	1.57	-	low
	-0.73	-	low

Section 12. Ecological information

ID 2 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 :

1H S/N	No known significant effects or critical hazards.
4Hz 0.1% H ₂ O/D ₂ O	No known significant effects or critical hazards.
Temp Grad	No known significant effects or critical hazards.
1H Lineshape	No known significant effects or critical hazards.
13C S/N ASTM doped	No known significant effects or critical hazards.
ID 1	No known significant effects or critical hazards.
ID 2	No known significant effects or critical hazards.
Sucrose, NMR tested	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

Additional information : **Remarks**
De minimis quantities

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 : TSCA 8(a) PAIR: Acetonitrile
 Commerce control list precursor: Trimethyl phosphite
 United States inventory (TSCA 8b): Not determined.
 Clean Water Act (CWA) 307: (²H)Chloroform; Ethylbenzene; Chromium(III) 4-oxopent-2-ene-2-olate; (²H₆)Benzene; Trichloromethane; Acetonitrile
 Clean Water Act (CWA) 311: (²H)Chloroform; Ethylbenzene; (²H₆)Benzene; Trichloromethane

Clean Air Act (CAA) 112 regulated toxic substances: (²H)Chloroform

Clean Air Act Section 112 (b) Hazardous Air Pollutants (HAPs) : 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) : Listed

[SARA 302/304](#)

[Composition/information on ingredients](#)

Name	%	EHS	SARA 302 TPQ		SARA 304 RQ	
			(lbs)	(gallons)	(lbs)	(gallons)
1H S/N (² H)Chloroform	60 - 100	Yes.	-	-	-	-
1H Lineshape Trichloromethane	0.1 - 1	Yes.	10000	803.8	10	0.8
ID 1 (² H)Chloroform	60 - 100	Yes.	-	-	-	-
Sucrose, NMR tested Sodium azide	< 0.1	Yes.	500	-	1000	-

SARA 304 RQ : 8000 lbs / 3632 kg

[SARA 311/312](#)

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

[Composition/information on ingredients](#)

Section 15. Regulatory information

Name	%	Fire hazard	Sudden release of pressure	Reactive	Immediate (acute) health hazard	Delayed (chronic) health hazard
1H S/N (² H)Chloroform Ethylbenzene	60 - 100 < 0.1	No. Yes.	No. No.	No. No.	Yes. Yes.	Yes. Yes.
1H Lineshape (² H ₆)Acetone Trichloromethane	60 - 100 0.1 - 1	Yes. No.	No. No.	No. No.	Yes. Yes.	No. Yes.
13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	30 - 60 30 - 60	Yes. Yes.	No. No.	No. No.	Yes. Yes.	Yes. Yes.
ID 1 (² H)Chloroform Iodomethane (¹³ C) Trimethyl phosphite	60 - 100 0.1 - 1 0.1 - 1	No. No. Yes.	No. No. No.	No. No. No.	Yes. Yes. Yes.	Yes. Yes. No.
ID 2 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	1H S/N (² H)Chloroform Ethylbenzene	865-49-6 100-41-4	60 - 100 0.1 - 1
	1H Lineshape Trichloromethane	67-66-3	0.1 - 1
	13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	1076-43-3 123-91-1	30 - 60 15 - 40
	ID 1 (² H)Chloroform Iodomethane (¹³ C)	865-49-6 4227-95-6	60 - 100 0.1 - 1
	ID 2 Benzamide (¹⁵ N)	31656-62-9	1 - 5
Supplier notification	1H S/N (² H)Chloroform Ethylbenzene	865-49-6 100-41-4	60 - 100 <0.1
	1H Lineshape Trichloromethane	67-66-3	0.1 - 1
	13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	1076-43-3 123-91-1	30 - 60 15 - 40
	ID 1 (² H)Chloroform	865-49-6	60 - 100

Section 15. Regulatory information

	Iodomethane (¹³ C)	4227-95-6	0.1 - 1
	ID 2 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

: The following components are listed: CHLOROFORM; 1,4-DIOXANE; BENZENE; ACETONE

New York

: The following components are listed: Chloroform; Methane, trichloro-; 1,4-Dioxane; Benzene; Acetone; 2-Propanone; Chloroform; Methane, trichloro-

New Jersey

: The following components are listed: CHLOROFORM; METHANE, TRICHLORO-; DIMETHYL SULFOXIDE; METHANE, SULFINYLBI-; 1,4-DIOXANE; 1, 4-DIETHYLENE DIOXIDE; BENZENE; ACETONE; 2-PROPANONE; CHLOROFORM; METHANE, TRICHLORO-

Pennsylvania

: The following components are listed: METHANE, TRICHLORO-; di[(²H₃)Methyl] sulphoxide; 1,4-DIOXANE; BENZENE; 2-PROPANONE; METHANE, TRICHLORO-

California Prop. 65

WARNING: This product contains a chemical known to the State of California to cause cancer and birth defects or other reproductive harm.

Ingredient name	Cancer	Reproductive	No significant risk level	Maximum acceptable dosage level
1H S/N (² H)Chloroform	Yes.	Yes.	20 µg/day (ingestion) 40 µg/day (inhalation)	No.
Ethylbenzene	Yes.	No.	41 µg/day (ingestion) 54 µg/day (inhalation)	No.
1H Lineshape Trichloromethane	Yes.	Yes.	20 µg/day (ingestion) 40 µg/day (inhalation)	No.
13C S/N ASTM doped (² H ₆)Benzene	Yes.	Yes.	6.4 µg/day (ingestion) 13 µg/day (inhalation)	24 µg/day (ingestion) 49 µg/day (inhalation)
1,4-Dioxane	Yes.	No.	Yes.	No.
ID 1 (² H)Chloroform	Yes.	Yes.	20 µg/day (ingestion) 40 µg/day (inhalation)	No.
Iodomethane (¹³ C)	Yes.	No.	No.	No.

Canada inventory

: Not determined.

International regulations

Section 15. Regulatory information

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	: 29/01/2014.
Date of previous issue	: No previous validation.
Version	: 3

✔ Indicates information that has changed from previously issued version.

Notice to reader

Disclaimer: The information contained in this document is based on Agilent's state of knowledge at the time of preparation. No warranty as to its accurateness, completeness or suitability for a particular purpose is expressed or implied.