Safety Data Sheet
acc. to OSHA HCS

Printing date 06/14/2024 *Reviewed on 06/14/2024*

1 Identification

· **Product identifier**

· **Trade name: 50% ACN + 47.5% H_2O + 2.5% TFA v/v**

· **Article number:** FIS026

· **Details of the supplier of the safety data sheet**
· **Manufacturer/Supplier:**
Aqua Solutions, Inc.
6913 Highway 225
DEER PARK, TX 77536
USA
800-256-2586

· **Information department:**
Technical Coordinator
Sherman Nelson shermann@aquasolutions.org
· **Emergency telephone number:**
Chemtrec: 800-424-9300
Canutec: 613-996-6666

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2 Hazard(s) identification

· **Classification of the substance or mixture**

GHS02 Flame

Flammable Liquids 2 H225 Highly flammable liquid and vapor.

GHS05 Corrosion

Skin Corrosion 1A H314 Causes severe skin burns and eye damage.
Eye Damage 1 H318 Causes serious eye damage.

GHS07

Acute Toxicity - Oral 4 H302 Harmful if swallowed.

· **Label elements**
· **GHS label elements** The product is classified and labeled according to the Globally Harmonized System (GHS).
· **Hazard pictograms**

GHS02 GHS05 GHS07

· **Signal word** Danger

· **Hazard-determining components of labeling:**
Acetonitrile, Reagent ACS Grade
Trifluoroacetic Acid
· **Hazard statements**
Highly flammable liquid and vapor.

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Harmful if swallowed.
Causes severe skin burns and eye damage.
· **Precautionary statements**
Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
Keep container tightly closed.
Ground/bond container and receiving equipment.
Use explosion-proof electrical/ventilating/lighting/equipment.
Use only non-sparking tools.
Take precautionary measures against static discharge.
Do not breathe dusts or mists.
Wash thoroughly after handling.
Do not eat, drink or smoke when using this product.
Wear protective gloves/protective clothing/eye protection/face protection.
If swallowed: Call a poison center/doctor if you feel unwell.
If swallowed: Rinse mouth. Do NOT induce vomiting.
If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
IF INHALED: Remove person to fresh air and keep comfortable for breathing.
If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Immediately call a poison center/doctor.
Specific treatment (see on this label).
Wash contaminated clothing before reuse.
In case of fire: Use CO2, powder or water spray to extinguish.
Store in a well-ventilated place. Keep cool.
Store locked up.
Dispose of contents/container in accordance with local/regional/national/international regulations.
· **Classification system:**
· **NFPA ratings (scale 0 - 4)**

Health = 3
Fire = 3
Reactivity = 0

· **HMIS-ratings (scale 0 - 4)**

*Health = *3*
Fire = 3
Reactivity = 0

· **Other hazards**
· **Results of PBT and vPvB assessment**
· **PBT:** *Not applicable.*
· **vPvB:** *Not applicable.*

3 Composition/information on ingredients

· **Chemical characterization: Mixtures**
· **Description:** *Mixture of the substances listed below with nonhazardous additions.*

· **Dangerous components:**		
CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	43.296%
CAS: 76-05-1	Trifluoroacetic Acid	4.121%

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· **Table of Nonhazardous Ingredients**

CAS: 7732-18-5	Water	52.584%

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4 First-aid measures

· **Description of first aid measures**
· **General information:**
Immediately remove any clothing soiled by the product.
Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.
· **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.
· **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
· **After eye contact:** Rinse opened eye for several minutes under running water. Then consult a doctor.
· **After swallowing:**
Immediately call a doctor.
Drink copious amounts of water and provide fresh air. Immediately call a doctor.
· **Information for doctor:**
· **Most important symptoms and effects, both acute and delayed** No further relevant information available.
· **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

· **Extinguishing media**
· **Suitable extinguishing agents:**
CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
· **Special hazards arising from the substance or mixture**
During heating or in case of fire poisonous gases are produced.
· **Advice for firefighters**
· **Protective equipment:** Mouth respiratory protective device.

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6 Accidental release measures

· **Personal precautions, protective equipment and emergency procedures**
Mount respiratory protective device.
Wear protective equipment. Keep unprotected persons away.
· **Environmental precautions:**
Dilute with plenty of water.
Do not allow to enter sewers/ surface or ground water.
· **Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Use neutralizing agent.
Dispose contaminated material as waste according to section 13.
Ensure adequate ventilation.
· **Reference to other sections**
See Section 7 for information on safe handling.
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

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· **Protective Action Criteria for Chemicals**

· **PAC-1:**		
CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	13 ppm
CAS: 76-05-1	Trifluoroacetic Acid	0.13 ppm

· **PAC-2:**		
CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	50 ppm
CAS: 76-05-1	Trifluoroacetic Acid	73 mg/m3

· **PAC-3:**		
CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	150 ppm
CAS: 76-05-1	Trifluoroacetic Acid	440 mg/m3

7 Handling and storage

· **Handling:**
· **Precautions for safe handling**
Ensure good ventilation/exhaustion at the workplace.
Prevent formation of aerosols.
· **Information about protection against explosions and fires:**
Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
Keep respiratory protective device available.

· **Conditions for safe storage, including any incompatibilities**
· **Storage:**
· **Requirements to be met by storerooms and receptacles:** Store in a cool location.
· **Information about storage in one common storage facility:** Not required.
· **Further information about storage conditions:**
Keep receptacle tightly sealed.
Store in cool, dry conditions in well sealed receptacles.
· **Specific end use(s)** No further relevant information available.

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8 Exposure controls/personal protection

· **Additional information about design of technical systems:** No further data; see section 7.

· **Control parameters**
· **Components with limit values that require monitoring at the workplace:**
The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.
At this time, the remaining constituent has no known exposure limits.

CAS: 75-05-8 Acetonitrile, Reagent ACS Grade	
PEL	Long-term value: 70 mg/m³, 40 ppm
REL	Long-term value: 34 mg/m³, 20 ppm
TLV	Long-term value: 20 ppm Skin, A4

· **Additional information:** The lists that were valid during the creation were used as basis.

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· **Exposure controls**
· **Personal protective equipment:**
· **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing.
Wash hands before breaks and at the end of work.
Avoid contact with the eyes.
Avoid contact with the eyes and skin.
· **Breathing equipment:**
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.
· **Protection of hands:**

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.
Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.
Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation
· **Material of gloves**
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.
· **Penetration time of glove material**
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
· **Eye protection:**

Tightly sealed goggles

· **Body protection:** Protective work clothing

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9 Physical and chemical properties

· **Information on basic physical and chemical properties**	
· **General Information**	
· **Appearance:**	
Form:	Liquid
Color:	Clear
· **Odor:**	Characteristic
· **Odor threshold:**	Not determined.
· **pH-value at 20 °C (68 °F):**	<2
· **Change in condition**	
Melting point/Melting range:	Undetermined.
Boiling point/Boiling range:	100 °C (212 °F)
· **Flash point:**	5 °C (41 °F)

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· **Flammability (solid, gaseous):**	Highly flammable.
· **Auto igniting:**	525 °C (977 °F)
· **Decomposition temperature:**	Not determined.
· **Ignition temperature:**	Product is not selfigniting.
· **Danger of explosion:**	Product is not explosive. However, formation of explosive air/vapor mixtures are possible.
· **Explosion limits:**	
Lower:	4.4 Vol %
Upper:	16 Vol %
· **Vapor pressure at 20 °C (68 °F):**	97 hPa (72.8 mm Hg)
· **Density at 20 °C (68 °F):**	0.92585 g/cm³ (7.72622 lbs/gal)
· **Relative density**	Not determined.
· **Vapor density**	Not determined.
· **Evaporation rate**	Not determined.
· **Solubility in / Miscibility with**	
Water:	Fully miscible.
· **Partition coefficient (n-octanol/water):**	Not determined.
· **Viscosity:**	
Dynamic:	Not determined.
Kinematic:	Not determined.
· **Solvent content:**	
Organic solvents:	4.1 %
Water:	52.6 %
VOC content:	4.12 % 38.2 g/l / 0.32 lb/gal
Solids content:	0.0 %
· **Other information**	No further relevant information available.

10 Stability and reactivity

· **Reactivity** No further relevant information available.
· **Chemical stability**
· **Thermal decomposition / conditions to be avoided:** No decomposition if used according to specifications.
· **Possibility of hazardous reactions** No dangerous reactions known.
· **Conditions to avoid** No further relevant information available.
· **Incompatible materials:** No further relevant information available.
· **Hazardous decomposition products:** No dangerous decomposition products known.

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11 Toxicological information

· **Information on toxicological effects**
· **Acute toxicity:**

· LD/LC50 values that are relevant for classification:		
ATE (Acute Toxicity Estimate)		
Oral	LD50	1,155 mg/kg
Dermal	LD50	2,541 mg/kg
Inhalative	LC50/4h	23.2 mg/l

· **Primary irritant effect:**
· **on the skin:** Strong caustic effect on skin and mucous membranes.
· **on the eye:**
Strong caustic effect.
Strong irritant with the danger of severe eye injury.
· **Sensitization:** No sensitizing effects known.
· **Additional toxicological information:**
The product shows the following dangers according to internally approved calculation methods for preparations:
Harmful
Corrosive
Irritant
Swallowing will lead to a strong caustic effect on mouth and throat and to the danger of perforation of esophagus and stomach.

· **Carcinogenic categories**

· IARC (International Agency for Research on Cancer)
None of the ingredients is listed.

· NTP (National Toxicology Program)
None of the ingredients is listed.

· OSHA-Ca (Occupational Safety & Health Administration)
None of the ingredients is listed.

12 Ecological information

· **Toxicity**
· **Aquatic toxicity:** No further relevant information available.
· **Persistence and degradability** No further relevant information available.
· **Behavior in environmental systems:**
· **Bioaccumulative potential** No further relevant information available.
· **Mobility in soil** No further relevant information available.
· **Additional ecological information:**
· **General notes:**
Water hazard class 2 (Self-assessment): hazardous for water
Do not allow product to reach ground water, water course or sewage system.
Must not reach bodies of water or drainage ditch undiluted or unneutralized.
Danger to drinking water if even small quantities leak into the ground.
Rinse off of bigger amounts into drains or the aquatic environment may lead to decreased pH-values. A low pH-value harms aquatic organisms. In the dilution of the use-level the pH-value is considerably increased, so that after the use of the product the aqueous waste, emptied into drains, is only low water-dangerous.
· **Results of PBT and vPvB assessment**
· **PBT:** Not applicable.

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· **vPvB:** Not applicable.
· **Other adverse effects** No further relevant information available.

13 Disposal considerations

· **Waste treatment methods**
· **Recommendation:**
Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

· **Uncleaned packagings:**
· **Recommendation:** Disposal must be made according to official regulations.
· **Recommended cleansing agent:** Water, if necessary with cleansing agents.

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14 Transport information

· **UN-Number**
· **DOT, IMDG, IATA** UN2924

· **UN proper shipping name**
· **DOT** Flammable liquids, corrosive, n.o.s. (acetonitrile, Trifluoroacetic Acid)
· **IMDG, IATA** FLAMMABLE LIQUID, CORROSIVE, N.O.S. (acetonitrile, Trifluoroacetic Acid)

· **Transport hazard class(es)**

· **DOT**

· **Class** 3 Flammable liquids
· **Label** 3, 8

· **IMDG**

· **Class** 3 Flammable liquids
· **Label** 3/8

· **IATA**

· **Class** 3 Flammable liquids
· **Label** 3 (8)

· **Packing group**
· **DOT, IMDG, IATA** II

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· **Environmental hazards:**	Not applicable.
· **Special precautions for user**	Warning: Flammable liquids
· **Hazard identification number (Kemler code):**	338
· **EMS Number:**	F-E,S-C
· **Segregation groups**	(SGG1) Acids
· **Stowage Category**	B
· **Stowage Code**	SW2 Clear of living quarters.
· **Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code**	Not applicable.
· **Transport/Additional information:**	
· **DOT**	
· **Quantity limitations**	On passenger aircraft/rail: 1 L On cargo aircraft only: 5 L
· **IMDG**	
· **Limited quantities (LQ)**	1L
· **Excepted quantities (EQ)**	Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· **UN "Model Regulation":**	UN 2924 FLAMMABLE LIQUID, CORROSIVE, N.O.S. (ACETONITRILE, TRIFLUOROACETIC ACID), 3 (8), II

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15 Regulatory information

· **Safety, health and environmental regulations/legislation specific for the substance or mixture**
No further relevant information available.
· **Sara**

· **Section 355 (extremely hazardous substances):**
None of the ingredients is listed.

· **Section 313 (Specific toxic chemical listings):**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade

· **TSCA (Toxic Substances Control Act):**

Water	ACTIVE
Acetonitrile, Reagent ACS Grade	ACTIVE
Trifluoroacetic Acid	ACTIVE

· **Hazardous Air Pollutants**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade

· **Proposition 65**

· **Chemicals known to cause cancer:**
None of the ingredients is listed.

· **Chemicals known to cause reproductive toxicity for females:**
None of the ingredients is listed.

· **Chemicals known to cause reproductive toxicity for males:**
None of the ingredients is listed.

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· **Chemicals known to cause developmental toxicity:**
None of the ingredients is listed.

· **Carcinogenic categories**

· **EPA (Environmental Protection Agency)**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	CBD, D

· **TLV (Threshold Limit Value)**

CAS: 75-05-8	Acetonitrile, Reagent ACS Grade	A4

· **NIOSH-Ca (National Institute for Occupational Safety and Health)**
None of the ingredients is listed.

· **GHS label elements** The product is classified and labeled according to the Globally Harmonized System (GHS).
· **Hazard pictograms**

GHS02 GHS05 GHS07

· **Signal word** Danger

· **Hazard-determining components of labeling:**
Acetonitrile, Reagent ACS Grade
Trifluoroacetic Acid
· **Hazard statements**
Highly flammable liquid and vapor.
Harmful if swallowed.
Causes severe skin burns and eye damage.
· **Precautionary statements**
Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
Keep container tightly closed.
Ground/bond container and receiving equipment.
Use explosion-proof electrical/ventilating/lighting/equipment.
Use only non-sparking tools.
Take precautionary measures against static discharge.
Do not breathe dusts or mists.
Wash thoroughly after handling.
Do not eat, drink or smoke when using this product.
Wear protective gloves/protective clothing/eye protection/face protection.
If swallowed: Call a poison center/doctor if you feel unwell.
If swallowed: Rinse mouth. Do NOT induce vomiting.
If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.
IF INHALED: Remove person to fresh air and keep comfortable for breathing.
If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Immediately call a poison center/doctor.
Specific treatment (see on this label).
Wash contaminated clothing before reuse.
In case of fire: Use CO2, powder or water spray to extinguish.
Store in a well-ventilated place. Keep cool.
Store locked up.
Dispose of contents/container in accordance with local/regional/national/international regulations.

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· **Chemical safety assessment:** A Chemical Safety Assessment has not been carried out.

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16 Other information

This information is based on our present knowledge. However, this shall not constitute a guarantee for any specific product features and shall not establish a legally valid contractual relationship.

· **Department issuing SDS:** Environment protection department.
· **Contact:**
Date of Preparation / Last Revision:
· **Date of preparation / last revision**
Revision 0.1, 06/14/2024: Reviewed SDS for accuracy. MH/STN
Revision 0.0, 05-29-2024: Creation date for SDS. STN
06/14/2024 / 1.0
· **Abbreviations and acronyms:**
IMDG: International Maritime Code for Dangerous Goods
DOT: US Department of Transportation
IATA: International Air Transport Association
EINECS: European Inventory of Existing Commercial Chemical Substances
ELINCS: European List of Notified Chemical Substances
CAS: Chemical Abstracts Service (division of the American Chemical Society)
NFPA: National Fire Protection Association (USA)
HMIS: Hazardous Materials Identification System (USA)
VOC: Volatile Organic Compounds (USA, EU)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
PBT: Persistent, Bioaccumulative and Toxic
vPvB: very Persistent and very Bioaccumulative
NIOSH: National Institute for Occupational Safety
OSHA: Occupational Safety & Health
TLV: Threshold Limit Value
PEL: Permissible Exposure Limit
REL: Recommended Exposure Limit
Flammable Liquids 2: Flammable liquids – Category 2
Acute Toxicity - Oral 4: Acute toxicity – Category 4
Skin Corrosion 1A: Skin corrosion/irritation – Category 1A
Eye Damage 1: Serious eye damage/eye irritation – Category 1
· *** Data compared to the previous version altered.**