

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Version 7.0

Revision Date 08.08.2023

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Dichloroacetic acid for synthesis

Product Number : 8.03541  
Catalogue No. : 803541  
Brand : Millipore  
Index-No. : 607-066-00-5  
REACH No. : 01-2120767065-52-XXXX  
CAS-No. : 79-43-6

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

Identified uses : Chemical for synthesis

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Chemie GmbH  
Eschenstrasse 5  
D-82024 TAUFKIRCHEN

Telephone : +49 (0)89 6513-1130  
Fax : +49 (0)89 6513-1161  
E-mail address : technischerservice@merckgroup.com

**1.4 Emergency telephone**

Emergency Phone # : 0800 181 7059 (CHEMTREC Deutschland)  
+49 (0)696 43508409 (CHEMTREC  
weltweit)

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****Classification according to Regulation (EC) No 1272/2008**

Corrosive to Metals (Category 1), H290  
Acute toxicity, Dermal (Category 3), H311  
Skin corrosion (Category 1), H314  
Serious eye damage (Category 1), H318  
Carcinogenicity (Category 2), H351  
Reproductive toxicity (Category 1B), H360FD  
Effects on or via lactation, H362



Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335  
Specific target organ toxicity - repeated exposure, Oral (Category 2), Brain, Liver, Testes, H373

Short-term (acute) aquatic hazard (Category 1), H400

Long-term (chronic) aquatic hazard (Category 3), H412

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

## 2.2 Label elements

### Labelling according Regulation (EC) No 1272/2008

Pictogram



Signal Word

Danger

Hazard statement(s)

H290

May be corrosive to metals.

H311

Toxic in contact with skin.

H314

Causes severe skin burns and eye damage.

H335

May cause respiratory irritation.

H351

Suspected of causing cancer.

H360FD

May damage fertility. May damage the unborn child.

H362

May cause harm to breast-fed children.

H373

May cause damage to organs (Brain, Liver, Testes) through prolonged or repeated exposure if swallowed.

H410

Very toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P263

Avoid contact during pregnancy and while nursing.

P273

Avoid release to the environment.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

P303 + P361 + P353

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.

P304 + P340 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard Statements

none

### Reduced Labeling (<= 125 ml)

Pictogram



Signal Word

Danger

Hazard statement(s)

H311

Toxic in contact with skin.

H351

Suspected of causing cancer.

H362

May cause harm to breast-fed children.

H314

Causes severe skin burns and eye damage.



H360FD	May damage fertility. May damage the unborn child.
Precautionary statement(s) P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
Supplemental Hazard Statements	none

### 2.3 Other hazards

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

#### Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

#### Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula	: C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> O <sub>2</sub>
Molecular weight	: 128,94 g/mol
CAS-No.	: 79-43-6
EC-No.	: 201-207-0
Index-No.	: 607-066-00-5

Component	Classification	Concentration
<b>Dichloroacetic Acid</b>		
CAS-No.	79-43-6	<= 100 %
EC-No.	201-207-0	
Index-No.	607-066-00-5	
		Met. Corr. 1; Acute Tox. 3; Skin Corr. 1A; Eye Dam. 1; Carc. 2; Repr. 1B; Lact. ; STOT RE 2; Aquatic Acute 1; H290, H311, H314, H318, H351, H360FD, H362, H373, H400



<b>Trichloroacetic acid</b>			
CAS-No.	76-03-9	Skin Corr. 1A; Eye Dam. 1; Aquatic Acute 1; Aquatic Chronic 1; H314, H318, H400, H410 Concentration limits: >= 1 %: STOT SE 3, H335;	>= 1 - < 2,5 %
EC-No.	200-927-2		
Index-No.	607-004-00-7		
<b>chloroacetic acid</b>			
CAS-No.	79-11-8	Acute Tox. 3; Skin Corr. 1B; Eye Dam. 1; STOT SE 3; Aquatic Acute 1; H301, H331, H311, H314, H318, H335, H400 Concentration limits: >= 5 %: STOT SE 3, H335; M-Factor - Aquatic Acute: 10	>= 0,1 - < 0,25 %
EC-No.	201-178-4		
Index-No.	607-003-00-1		

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

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

#### In case of eye contact

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

#### If swallowed

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

### 4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

### 4.3 Indication of any immediate medical attention and special treatment needed

No data available



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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

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

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Hydrogen chloride gas

Combustible.

Fire may cause evolution of:

Hydrogen chloride gas

Phosgene

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

### 5.4 Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

### 6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

#### Advice on safe handling

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Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

### **Hygiene measures**

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

For precautions see section 2.2.

## **7.2 Conditions for safe storage, including any incompatibilities**

### **Storage conditions**

No metal or light-weight-metal containers. No metal containers.

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Recommended storage temperature see product label.

### **Storage class**

Storage class (TRGS 510): 6.1C: Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects

## **7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## **SECTION 8: Exposure controls/personal protection**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

### **8.2 Exposure controls**

#### **Personal protective equipment**

##### **Eye/face protection**

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

##### **Skin protection**

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Viton®

Minimum layer thickness: 0,7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact



Material: Chloroprene  
Minimum layer thickness: 0,65 mm  
Break through time: 120 min  
Material tested:KCL 720 Camapren®

### **Body Protection**

Acid-resistant protective clothing

### **Respiratory protection**

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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

### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

a) Physical state	liquid
b) Color	colorless
c) Odor	pungent
d) Melting point/freezing point	Melting point/range: 13,5 °C
e) Initial boiling point and boiling range	193 - 195 °C at 1.013,25 hPa
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	No data available
h) Flash point	113 °C - closed cup
i) Autoignition temperature	No data available
j) Decomposition temperature	No data available
k) pH	1,2 at 129 g/l at 20 °C
l) Viscosity	Viscosity, kinematic: 4,696 mm <sup>2</sup> /s at 20 °C, 2,716 mm <sup>2</sup> /s at 40 °C  Viscosity, dynamic: No data available
m) Water solubility	soluble



- n) Partition coefficient: log Pow: 0,92 - (Lit.), Bioaccumulation is not expected.  
n-octanol/water
- o) Vapor pressure 0,19 hPa at 20 °C
- p) Density 1,567 g/cm<sup>3</sup> at 20 °C  
Relative density 1,56 at 20 °C
- q) Relative vapor density 4,45 - (Air = 1.0)
- r) Particle characteristics No data available
- s) Explosive properties No data available
- t) Oxidizing properties none

## 9.2 Other safety information

Relative vapor density 4,45 - (Air = 1.0)

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Risk of explosion with:  
furfuryl alcohol  
Violent reactions possible with:  
Amines  
Bases  
Strong oxidizing agents  
strong reducing agents  
Sulfur compounds  
Risk of ignition or formation of inflammable gases or vapours with:  
Metals  
mercaptans  
Exothermic reaction with:  
Water

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Acute toxicity estimate Oral - > 2.000 mg/kg

(Calculation method)

LD50 Oral - Rat - 2.820 mg/kg (Dichloroacetic Acid)

(OECD Test Guideline 401)

Acute toxicity estimate Inhalation - 4 h - > 5 mg/l - dust/mist(Calculation method)

Acute toxicity estimate Dermal - 808,95 mg/kg

(Calculation method)

LD50 Dermal - Rabbit - 797 mg/kg (Dichloroacetic Acid)

Remarks: (ECHA)

Acute toxicity estimate Dermal - 797 mg/kg (Dichloroacetic Acid)

(Calculation method)

#### Skin corrosion/irritation

Skin - Rabbit (Dichloroacetic Acid)

Result: Causes severe burns.

Remarks: (RTECS)

#### Serious eye damage/eye irritation

Eyes - Rabbit (Dichloroacetic Acid)

Result: Causes serious eye damage.

Remarks: (RTECS)

Remarks: Causes serious eye damage.

#### Respiratory or skin sensitization

No data available

#### Germ cell mutagenicity

Test Type: In vitro mammalian cell gene mutation test

(Dichloroacetic Acid)

Test system: mouse lymphoma cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

Test Type: Ames test

(Dichloroacetic Acid)

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

(Dichloroacetic Acid)

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

(Dichloroacetic Acid)



Test Type: Transgenic rodent somatic cell gene mutation assay  
Species: Mouse  
Cell type: Liver cells  
Application Route: Oral

Result: negative  
Remarks: (ECHA)  
(Dichloroacetic Acid)  
Test Type: Micronucleus test  
Species: Rat  
Cell type: Bone marrow  
Application Route: Oral  
Method: OECD Test Guideline 475  
Result: negative

#### **Carcinogenicity**

Suspected of causing cancer. (Dichloroacetic Acid)

#### **Reproductive toxicity**

May damage the unborn child. (Dichloroacetic Acid)  
May damage fertility. Studies indicating a hazard to babies during the lactation period (Dichloroacetic Acid)

#### **Specific target organ toxicity - single exposure**

No data available

#### **Specific target organ toxicity - repeated exposure**

Oral - May cause damage to organs through prolonged or repeated exposure.  
- Brain, Liver, Testes

#### **Aspiration hazard**

No data available

### **11.2 Additional Information**

#### **Endocrine disrupting properties**

##### **Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., Cough, Shortness of breath, Headache, Nausea (Dichloroacetic Acid)  
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. (Dichloroacetic Acid)

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

No data available



## 12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 15 d (Dichloroacetic Acid)  
Result: 93 % - Readily biodegradable.  
(OECD Test Guideline 301F)

## 12.3 Bioaccumulative potential

No data available

## 12.4 Mobility in soil

No data available

## 12.5 Results of PBT and vPvB assessment

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

## 12.6 Endocrine disrupting properties

### Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

## 12.7 Other adverse effects

Forms corrosive mixtures with water even if diluted.  
Discharge into the environment must be avoided.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 1764    IMDG: 1764    IATA: 1764

### 14.2 UN proper shipping name

ADR/RID: DICHLOROACETIC ACID  
IMDG: DICHLOROACETIC ACID  
IATA: Dichloroacetic acid

### 14.3 Transport hazard class(es)

ADR/RID: 8    IMDG: 8    IATA: 8

### 14.4 Packaging group

ADR/RID: II    IMDG: II    IATA: II

### 14.5 Environmental hazards

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



## 14.6 Special precautions for user

Tunnel restriction code : (E)

Further information : No data available

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## SECTION 15: Regulatory information

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

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

#### Authorisations and/or restrictions on use

##### National legislation

Seveso III: Directive 2012/18/EU of the E1 ENVIRONMENTAL HAZARDS  
European Parliament and of the Council  
on the control of major-accident hazards  
involving dangerous substances.

##### Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

### 15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

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## SECTION 16: Other information

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

H290	May be corrosive to metals.
H301	Toxic if swallowed.
H311	Toxic in contact with skin.
H314	Causes severe skin burns and eye damage.
H318	Causes serious eye damage.
H331	May be corrosive to metals.
H335	Toxic in contact with skin.
H351	Causes severe skin burns and eye damage.
H360FD	Suspected of causing cancer.
H362	May damage fertility. May damage the unborn child.
H373	May cause harm to breast-fed children.
H400	May cause damage to organs (Brain, Liver, Testes) through prolonged or repeated exposure if swallowed.
H410	Very toxic to aquatic life.
H412	Toxic if inhaled.

### Relevant changes since previous version

2. Hazards identification



## Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

## Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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