



KATHON™ CG

A Safe, Effective, Globally Approved Preservative for Rinse-Off Products

Features, Benefits and Applications

Rohm and Haas discovered the active ingredients of KATHON CG preservative in the late 1960s. For over thirty years we have driven the progress of isothiazolinone chemistry to meet your evolving needs. Our goal is to provide our personal care customers with much more than a preservative. Rohm and Haas is committed to both the isothiazolinone chemistry and the personal care industry. We have extensive toxicological and environmental databases and internal expertise that has allowed KATHON CG to be registered globally, including Japan. This knowledge has also helped us support the product with both dermatologists and regulatory authorities throughout the world with the following services:

- Regulatory data
- Extensive toxicological databases
- Environmental fate database that is continually updated
- Safe handling expertise that can help you in your manufacturing facilities
- Technical expertise with isothiazolinone chemistry
- More than 100 patents obtained since the 1960s
- Public relations/media expertise and support

Features and Benefits

- Lowest dose
- Broader spectrum of activity
- Worldwide registrations, including Japan
- Supplied as an aqueous solution readily incorporated into cosmetic formulations
- Good compatibility with surfactants and emulsifiers, irrespective of their ionic nature
- Effective over the entire pH range normally encountered in cosmetics
- No color or odor imparted to cosmetic products
- Low toxicity at recommended use levels
- Environmentally acceptable
- Rapidly biodegradable
- Non-persistent in the environment
- Not bioaccumulating

Applications

- Body washes
- Conditioners
- Liquid Soaps
- Shampoos
- Wipes

Physical and Chemical Characteristics

Chemical Identification

The active ingredients of KATHON CG preservative are two isothiazolinones, identified by the IUPAC system of nomenclature as: 5-chloro-2-methyl-4-isothiazolin-3-one and 2-methyl-4-isothiazolin-3-one.

CTFA/INCI Name	CAS Number	Empirical Formula
Active Ingredients:		
Methyl chloro isothiazolinone	26172-55-4	C ₄ H ₄ Cl NOS
Methyl isothiazolinone	2682-20-4	C ₄ H ₅ NOS
The INCI Name Includes the Additional Ingredients:		
Magnesium chloride	7786-30-3	Mg Cl ₂
Magnesium nitrate	10377-60-3	Mg (NO ₃) ₂

Typical Properties

KATHON CG preservative is a precise formulation of active ingredients and inert salts in an aqueous solution. Each batch of KATHON CG is manufactured to exact specifications and a certificate of analysis can be provided with each order.

Miscibility

KATHON CG is totally miscible in water, lower alcohols and glycols and has low solubility in hydrocarbons.

KATHON CG	
Active Ingredients:	
5-chloro-2-methyl-4-isothiazolin-3-one	1.15%
2-methyl-4-isothiazolin-3-one	0.35%
Total	1.50%
Inert Ingredients:	
Magnesium salts (chloride and nitrate)	23.00%
Water	to 100.00%

Typical Physical Properties

These properties are typical but do not constitute specifications.

Appearance	Clear liquid
Color	APHA ≤ 100
Odor	Mild
Specific gravity @ 25°C	1.21
pH (as manufactured)	1.7 - 3.7
Stability	Stable at least one year at ambient temperatures and at least 6 months at 50°C

Recommended Use Directions

The maximum recommended use level for KATHON CG preservative is 0.1% by weight of product as supplied (15 parts per million active ingredient) in rinse-off products and 0.05% (7.5 parts per million active ingredient) in leave-on products. Because the components of personal care formulations vary considerably and may have an impact on the effect of preservatives, we urge each manufacturer to confirm the efficacy and stability of KATHON CG in use.

Microbiological Properties

KATHON CG preservative exhibits outstanding antimicrobial activity against Gram-positive and Gram-negative bacteria, molds and yeasts. The following table gives the minimum level in ppm of KATHON CG, as supplied, and as active ingredient that inhibited the growth of various microorganisms in test tube cultures.

The data demonstrate the broad spectrum activity of KATHON CG, but must not be taken as recommended use concentrations. Also, the microorganisms listed are not necessarily involved in the contamination of personal care products.

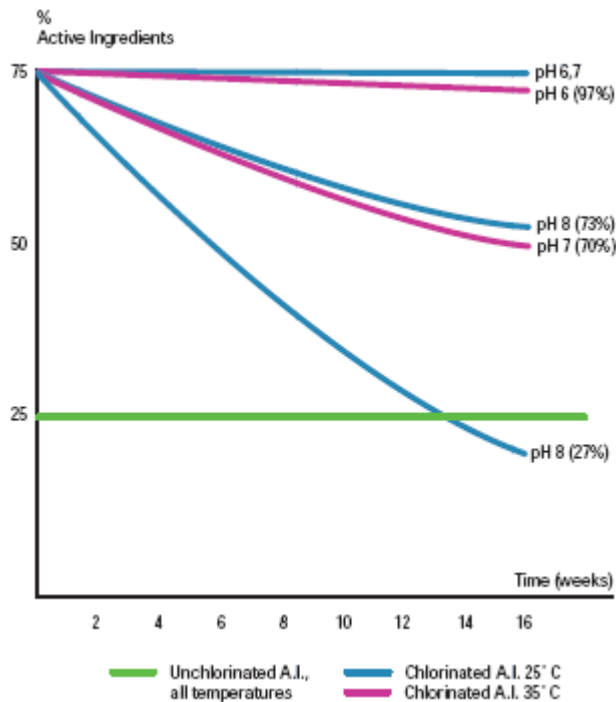
Organism	ATCC No.	KATHON CG (as supplied, ppm)	Active Ingredient (ppm)
Bacteria*			
Gram-Positive			
<i>Bacillus cereus var. mycoides</i>	(R&H No. L5)	150	2
<i>Bacillus subtilis</i>	(R&H No. B2)	150	2
<i>Brevibacterium ammoniagenes</i>	6871	150	2
<i>Sarcina lutea</i>	9341	300	5
<i>Staphylococcus aureus</i>	6538	150	2
<i>Staphylococcus epidermidis</i>	155	150	2
<i>Streptococcus pyogenes</i>	624	600	9
Gram-Negative			
<i>Achromobacter parvulus</i>	4335	150	2
<i>Alcaligenes faecalis</i>	8750	150	2
<i>Burkholderia (Pseudomonas) cepacia</i>	Gibraltar 165	50	0.75
<i>Enterobacter aerogenes</i>	3906	300	5
<i>Escherichia coli</i>	11229	300	5
<i>Flavobacterium suaveolens</i>	958	600	9
<i>Proteus vulgaris</i>	8427	300	5
<i>Pseudomonas aeruginosa</i>	15442	300	5
<i>Pseudomonas fluorescens</i>	13525	150	2
<i>Pseudomonas oleoverans</i>	8062	300	5
<i>Salmonella typhosa</i>	6539	300	5
<i>Shigella sonnei</i>	9292	150	2
Fungi*			
<i>Aspergillus niger</i>	9642	600	9
<i>Aspergillus oryzae</i>	10196	300	5
<i>Candida albicans</i> (yeast)	11651	300	5
<i>Chaetomium globosum</i>	6205	600	9
<i>Gliocladium fimbriatum</i>	(QM 7638)	600	9
<i>Mucor rouxii</i>	(R&H L5-83)	300	5
<i>Penicillium funiculosum</i>	9644	300	5
<i>Penicillium variable (glaucum)</i>	(U.S.D.A.)	150	2
<i>Phoma herbarum (pigmentivora)</i>	12569	150	2
<i>Pullularia (Aureobasidium) pullulans</i>	9348	300	5
<i>Rhizopus stolonifer</i>	10404	300	5
<i>Rhodotorula rubra</i> (yeast)	9449	150	2
<i>Saccharomyces cerevisiae</i> (yeast)	2601	150	2
<i>Trichophyton mentagrophytes (interdigitale)</i>	9533	300	5

* Bacteriostatic and fungistatic tests performed by serially diluting test compounds in trypticase soy broth and 1:100 inoculation with 24-hour broth cultures of the test bacterium or a fungal spore suspension prepared from 7-14 day culture slants washed with 7 ml of deionized water. Minimum inhibitory concentration levels determined visually after 2 days incubation at 37°C for bacteria and 28 to 30°C for fungi.

Chemical Stability

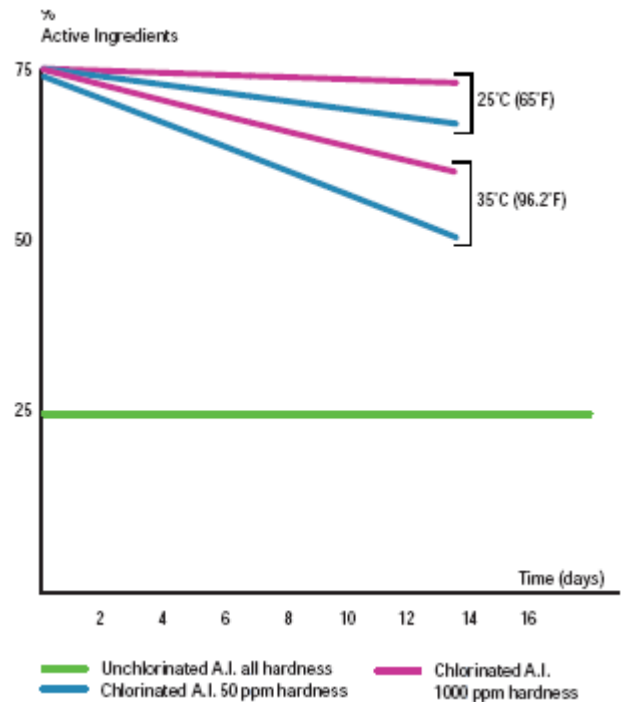
KATHON CG preservative has an established history of successful use as a preservative in personal care products. It has been shown to provide protection in a wide range of products over many years. However, there are some circumstances in which we would advise potential users to confirm preservative stability. These are outlined below, together with recommendations on how to optimize stability.

Figure 1: Stability of KATHON CG Preservative in Deionized Water versus pH at 25° and 35°C



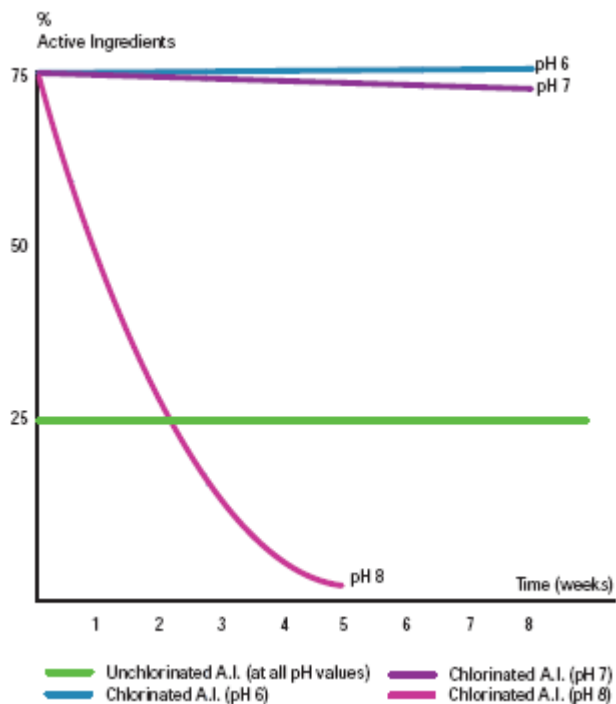
Temperatures and pH: As a general rule, a rise in temperature accelerates the rate of degradation of chemicals. As demonstrated in *Figure 1* above, KATHON CG is no exception. We recommend that temperatures in excess of 50°C should be avoided during manufacturing once the preservative has been incorporated into the formulation. Stability at ambient temperature is very much formulation dependent. Generally, KATHON CG is stable up to a pH of 8.0 over the lifetime of personal care products.

Figure 2: Stability of KATHON CG Preservative versus Water Hardness at pH 8



Water Hardness: The presence of calcium and magnesium in hard water has a significant positive impact on the stability of KATHON CG, as shown in *Figure 2* above. KATHON CG has been found to remain stable in the presence of hard water under circumstances in which breakdown would normally be anticipated.

Figure 3: Stability of KATHON CG Preservative in a 2.5% Cocamide Diethanolamine Aqueous Solution at 35°C and Various pH Values



Amines and Amine Derivatives: The presence of amine impurities in raw materials has a deleterious effect on the stability of KATHON CG. Secondary amines, in particular, show severe antagonism, but a simple reduction in pH to below 7, converting the amine to its acid salt, normally resolves the problem as demonstrated in *Figure 3* (opposite).

Reducing Agents: Some reducing agents are detrimental to isothiazolinone stability. Sulfated and sulfonated surfactants often contain residual sulfite or bisulfite, which can react with KATHON CG. We have found that use levels of the preservative are stable in the presence of up to about 25 ppm bisulfite (expressed as SO₂). Stability of KATHON CG in surfactants where the level is greater than 25 ppm can be optimized by treating the surfactant with a suitable oxidizing agent prior to adding KATHON CG.

Thiols: Thiols such as cysteine and zinc pyrithione are detrimental to the stability of KATHON CG preservative. Proteins or protein hydrolysates may contain thiols which could be available to react with KATHON CG.

Formulation Recommendations

Following our recommendations in formulating with KATHON CG preservative will enhance stability and control preservative cost.

It is important to follow these general guidelines when possible:

- Slightly acidic pH values are preferred
- Neutralize free diethanolamine when present (with citric acid for example)
- Eliminate residual SO₂ when present, using a suitable oxidizing agent
- Avoid high temperatures. During manufacture, add KATHON CG when the temperature is at or below 50°C
- Stearic and phosphoric acids can react with magnesium stabilizers in KATHON CG to form insoluble magnesium stearate and magnesium phosphate salts
- Use hard water (better than D.I.) when possible
- Avoid formulations in which cysteine and zinc pyrithione are present
- KATHON CG preservative stability should be evaluated in products containing protein hydrolysates to ensure preservative stability is adequate
- KATHON CG can be used effectively in combination with a wide range of preservatives

The information presented in this bulletin will help you evaluate KATHON CG as a preservative for your products. Rohm and Haas will be pleased to assist you in determining the optimum concentration of KATHON CG preservative for specific product formulations.

Efficacy in Cosmetics and Toiletries

The microbiological performance of KATHON CG preservative in most personal care products is excellent. Long-term microbiological protection is obtained employing use levels up to 15 ppm active ingredient (0.1% product, as supplied, by weight). Typical use levels for most personal care products (shampoos, conditioners, gels and surfactants) are in the range of 5 ppm to 10 ppm active ingredients (a.i.). For each formulation, it is important to insure stability of the active ingredient and assess the efficacy through a microbiological challenge test.

Rohm and Haas typically uses a 4-week challenge test with 2 inoculations of a mixed inoculum, coupled with an analysis of the active ingredient by High-Performance Liquid Chromatography (HPLC). More details of this procedure can be obtained from your nearest Rohm and Haas sales office.

For more information on the mechanism of action of KATHON CG, please request Rohm and Haas publication "*KATHON Biocides - Mechanism of Action.*"

Analytical Procedures

High-Performance Liquid Chromatography

HPLC analysis is the preferred method for determining low levels (0.01-0.1%) of KATHON CG preservative.

This method can be used to determine KATHON CG levels in many personal care products. If you require detailed information on HPLC methods, please contact your local Rohm and Haas sales office.

Toxicological Summary

The toxicology of the active ingredients of KATHON CG preservative has been assessed in extensive clinical and nonclinical testing, including acute and chronic toxicity tests, genotoxicity and dermal sensitization studies. Results of these studies have demonstrated that KATHON CG does not present a mutagenic, carcinogenic, or teratogenic risk to humans.

Like most cosmetic preservatives, at higher than recommended use level concentrations, KATHON CG preservative can cause contact dermatitis (skin irritation and/or skin sensitization). The use of KATHON CG at recommended use levels is safe. This is supported by our extensive toxicological and clinical databases, our work with dermatologists worldwide and many years of experience with safe use in a large number of personal care products worldwide.

Acute Toxicity

Oral LD ₅₀ (rat)	female	2630 mg/kg (product as sold)
	male	3350 mg/kg (product as sold)
Dermal LD ₅₀		>5000 mg/kg (product as sold)
Inhalation LC ₅₀ (rats) 4h	nose only	0.33 mg a.i./litre air
Skin irritation		Corrosive (product as sold)
Eye irritation		Corrosive - severe corneal damage (product as sold)
Sensitization		Skin sensitizer

Good Manufacturing Practices

A preservative is formulated into cosmetics and toiletries principally to protect the products from chance microbial challenge during production, storage and final customer use. It should not be expected to cope with severe contamination problems brought about by poor manufacturing practices. In the manufacturing plant, it is important that all potential sources of microbial contamination are identified and controlled.

Some of the important sources of microbial contamination include:

- Raw materials
- Water supplies
- Poor housekeeping and plant design
- Poor hygiene
- Inadequate cleaning and sanitization protocols
- Product reworking

Once identified, steps can be taken to control the level of contamination. Good manufacturing practices, backed up by regular and effective monitoring programs, are key factors. See Rohm and Haas publication "*Preventing Microbial Contamination in Manufacturing*."

Environmental Information

Environmental Toxicology

Rohm and Haas has extensive freshwater and marine ecotoxicity and environmental fate databases with all the necessary studies to perform a state-of-the-art environmental risk assessment.

Degradation and Dissipation in the Environment

In a series of experiments the modes and rates of dissipation and degradation in several ecosystems have been investigated including:

- Aquatic hydrolysis
- Bioaccumulation studies
- Soil leaching
- Photolysis
- Modes and rates of breakdown
- Dissipation in wastewater treatment plants
- River water die-away studies
- Degradative pathways
- Activated sludge respiration inhibition
- Soil dissipation

The above studies indicate that the active ingredients in KATHON CG are biodegradable and that the biocide degrades rapidly in the environment, producing harmless metabolites.

Environmental Risk Assessment

The risk associated with the use of a preservative depends not only on the hazard of the product, but also on the likelihood and extent of exposure. This can be established by performing an environmental risk assessment.

The environmental risk assessment using the results of the above studies demonstrates that KATHON CG preservative at normal use/dilution levels has minimal environmental impact because of the following properties:

- High-performance product used at very low levels
- Rapidly degraded to non-toxic, non-persistent substances
- Degradation does not produce chlorine or chlorinated organics
- Does not affect the performance of wastewater treatment plants
- Does not bioaccumulate
- Predicted environmental concentration (PEC) will have minimal environmental impact

For more information, please request publication "*KATHON CG, KATHON CG/ICP and KATHON CG/ICP II Preservatives Environmental Chemistry and Ecotoxicology*," or contact your local Rohm and Haas sales office.

Safe Handling Guidelines

You can count on Rohm and Haas personnel to provide you with advice and assistance on the safe handling of KATHON CG preservative in your plant. The following handling precautions should be observed with the product, as supplied:

Personal Protective Equipment

- **Material is CORROSIVE. Do not get in eyes, on skin, or clothing.** Causes eye damage and skin burns. May cause allergic skin reaction. May be harmful if swallowed or absorbed through the skin. Keep away from children.
- **Wear appropriate safety gear when handling.** Wear goggles or safety glasses, face shield and gloves (butyl rubber or nitrile) when handling. Avoid breathing vapor or mist. Avoid contamination of food. Do not take internally. Wash thoroughly after handling.

First Aid Measures

- **After contact with eyes:** FLUSH IMMEDIATELY with copious amounts of water for at least 15 minutes, with the eyes held open. Get prompt medical attention but FLUSH FIRST.
- **After contact with skin:** FLUSH IMMEDIATELY with plenty of water for at least 15 minutes. Remove and launder contaminated clothing. Wash affected skin thoroughly with soap and water. Wash thoroughly even if no skin burns are present since they may become apparent only after long contact time following inadequate washing.
- **If inhaled:** Remove casualty immediately to fresh air. If not breathing, apply artificial respiration. If breathing is difficult, give oxygen. Call a physician immediately.
- **If ingested:** Dilute the ingested product by giving water to drink. Call a physician at once. Never give anything by mouth to an unconscious person.

NOTE TO PHYSICIAN: Corrosive material. Probable mucosal damage may contraindicate the use of gastric lavage. It is inadvisable to induce vomiting. Measures against circulatory shock, respiratory depression, and convulsions may be needed.

Disposal of Spilled and Waste Material

Spills and cleaning runoffs should not be discharged where they can drain into sewage treatment plants, lakes, streams, ponds, or other public waters. Follow the disposal methods given on the package label and observe all federal, state, and local regulations.

KATHON CG preservative-containing wastes must not be discharged into public waters or sewage treatment systems. Such wastes must be deactivated (see below) and adequately diluted before discharge into any public water or sewage treatment facility. When considering disposal of any waste, observe all federal, state, and local regulations.

Deactivation Preparation of Equipment for Manufacturing

Deactivation - General

The active ingredients of KATHON CG preservative are readily deactivated or degraded to non-toxic components by the addition of a solution of 5% sodium hypochlorite (household bleach) and 5% sodium bicarbonate. Deactivation is typically accomplished by adding household bleach to the 3 quart (3 liters) fill mark on a 1 gallon (4 liters) plastic container containing 1/3 of a lb. (150 grams) of sodium bicarbonate. Close the container securely and shake well for 1 minute.

Estimate the volume of remaining spilled material. Apply 10 times the volume of deactivation solution per volume of spilled material remaining. The deactivation solution should remain in contact with KATHON CG for at least 30 minutes. The actual deactivation reaction takes place in much less time, but the added time ensures that the reaction goes to completion. Aqueous waste properly treated with deactivation solution can be discharged to the chemical sewer, if in accordance with federal, state, and local procedures, permits, and regulations.

The deactivation solution should be prepared fresh as needed since it gradually loses its effectiveness. Personnel making up or handling deactivation solutions should wear goggles or face shield, rubber apron and full-length butyl rubber or nitrile gloves, and a half face-piece respirator with organic vapor/acid gas cartridge and dust/mist prefilter (e.g., N-95 or higher efficiency, in the presence of oil mist, use R-95, P-95, or higher efficiency).

Deactivation - Preparation of Equipment for Maintenance

Mixing vessels, lines and pumps and other equipment containing residues of KATHON CG preservative must be deactivated before carrying out maintenance or repair work or using for other service. Drips, spills and exposed wet areas and valves should be cleaned up promptly with deactivation solution. To deactivate the surfaces of equipment, swab with deactivation solution, wait 30 minutes for the reaction to subside and rinse thoroughly with clean water. Rinse tools, pails, funnels and lines with water. To determine the amount of deactivation solution needed for cleanup, estimate the volume of KATHON CG preservative solution remaining in a well-drained system of vessels, lines and pumps, and make up and charge 10 volumes of deactivation solution per volume of preservative solution, then add more water to provide thorough mixing and contact throughout the equipment. Circulate the mixture through the system, allowing a reaction period of about 30 minutes, then drain and rinse with clean water or detergent solution. Drain to a municipal or chemical sewer if in accordance with federal, state, and local regulations.

Deactivation - Cleanup of Spills

Personnel cleaning up spills should wear appropriate protective clothing. This should include a rubber apron or impervious jacket, impervious full-length butyl rubber or nitrile gloves, footwear, chemical splash goggles and a half facepiece respirator with organic vapor/acid gas cartridge and dust/mist prefilter.

Please contact Rohm and Haas for information in the event of a major accidental spill.

Spilled material should be diked and absorbed on a spill control pillow or onto an inert solid such as clay or vermiculite. Shovel the absorbent and the soil beneath it to a depth sufficient to remove all preservative into a pail or drum. This material should then be disposed of in accordance with federal, state and local regulations; our recommended method of disposal is incineration.

Any residual KATHON CG preservative remaining on the spill site should then be treated with deactivation solution. A weight ratio of ten parts deactivation solution to one part KATHON CG should be used for this treatment. After allowing 30 minutes contact time, rinse the area with copious amounts of water and flush to the sewer, if in accordance with federal, state, and local regulations. For details please request publication "*KATHON CG, Spill Clean-Up and Deactivation Procedure.*"

Note: Do not add deactivation solution to the waste pail.

Material Safety Data Sheets

Material Safety Data Sheets (MSDS) are available for all Rohm and Haas products. These sheets contain pertinent information that you may need to protect your employees and customers against any known health and safety hazards associated with our products. We recommend that you obtain copies of our MSDS from your local Rohm and Haas technical representative before using our products in your facilities. We also suggest that you contact your suppliers of other materials recommended for use with our products for appropriate health and safety precautions before using them.

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Suggestions for uses of our products or the inclusion of descriptive material from patents and the citation of specific patents in this publication should not be understood as recommending the use of our products in violation of any patent or as permission or license to use any patent of the Rohm and Haas Company.

Material Safety Data Sheets outlining known health and safety hazards and handling methods for our products are available on request.



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