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TECHNICAL DATA SHEET

Product name: Cetrimonium Chloride

INCI name: Hexadecyltrimethylammonium chloride, Water

CAS: 112-02-7, 7732-18-5

Synonyms: Cetyltrimethylammonium Chloride

Chemical classification: Synthetic polymer, quaternary ammonium compound, mixture
Functional category: Hair conditioning agent

IUPAC name: N,N,N-Trimethylhexadecan-1-ammonium chloride

Chemical-physical properties: Cetrimonium chloride, also known as cetyltrimethylammonium chloride, is a chemical compound consisting of a cetyl alkyl chain ($C_{16}H_{33}$) attached to a trimethylammonium group ($(CH_3)_3N^+$) with a chloride anion (Cl^-). The cetyl alkyl chain is hydrophobic, allowing the molecule to interact with lipids and fatty substances, which is key to reducing static electricity and increasing hair shine. The trimethylammonium group, positively charged with three methyl groups attached to nitrogen, allows the molecule to bind to negatively charged surfaces, such as the hair surface. The cationic nature of this group helps neutralize the negative charge on the hair, reducing static electricity and facilitating hair combing. The chloride anion (Cl^-) balances the positive charge of the trimethylammonium group, making the structure stable. This combination of properties makes cetrimonium chloride very effective in hair care cosmetic products, especially in conditioners and hair rinses. The aqueous solution of cetrimonium chloride is a clear to slightly yellowish liquid with a mild odor. It has a viscosity that allows easy handling and mixing with other ingredients in formulations. The solution is stable over a wide pH range, important for various cosmetic applications. The substance is hygroscopic, meaning it can absorb moisture from the environment. The active component content is 25%. pH (2% solution) is 3 - 5.

Mechanism of action: Cetrimonium chloride is a quaternary ammonium salt with multiple functions in personal care products, including acting as a surfactant/emulsifier that cleans the skin by mixing water with dirt and oil. On the skin, cetrimonium chloride acts as a surfactant. Surfactants have hydrophilic and hydrophobic parts. When cetrimonium chloride is applied to the skin, the hydrophobic part of the molecule binds to oil and

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impurities on the skin's surface. The hydrophilic part binds to water. When we rinse the skin with water, micelles form - structures where oil and impurities are enclosed in the center, surrounded by the hydrophilic parts of the surfactant. This allows for effective removal of oil and impurities, leaving the skin clean and refreshed. In hair care products, cetrimonium chloride has conditioning properties. Its positively charged (cationic) structure allows it to bind to the negatively charged hair surface. This interaction helps smooth the hair surface and reduce friction between hair strands, resulting in reduced frizz and static electricity. Hair becomes smooth and silky, easier to comb and style. Additionally, cetrimonium chloride is used for its antimicrobial properties. It acts on microbes by disrupting the microorganism membranes, preventing their growth and reproduction. This helps prevent unwanted odors and extends the shelf life of cosmetic products. Due to its colorless to light yellow liquid form, it easily integrates into various formulations without changing the color or texture of the product.

Benefits:

- ***Effective cleansing:*** As a surfactant, cetrimonium chloride helps remove dirt, oil, and other impurities from the skin and hair. Its ability to bind water with oily particles allows thorough rinsing and cleansing of the skin.
- ***Hair conditioning:*** In hair care products, cetrimonium chloride acts as a conditioner that improves hair texture. It softens the hair, makes it smooth and easy to comb, reducing frizz and static electricity.
- ***Easier detangling:*** Reduces friction between hair strands, facilitating detangling, which is especially useful for people with long or curly hair.
- ***Antimicrobial properties:*** Cetrimonium chloride helps prevent the growth of microorganisms in cosmetic products. This extends the product's shelf life and prevents the development of unpleasant odors.
- ***Versatility:*** Can be included in various cosmetic formulations, from rinse-off to leave-on products, due to its compatibility with different ingredients.

Usage: For rinse-off products, concentrations up to 10% are recommended, while for leave-on products, concentrations from 0.25% to 1% are recommended to avoid irritation. Cetrimonium chloride can be added at different stages of cosmetic product manufacturing. If the product consists of multiple phases (e.g., oil and water phases), cetrimonium chloride can be added to the water phase before the phases are combined. In the case of emulsions (such as creams and lotions), cetrimonium chloride can be added after

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the oil and water phases have been mixed. The effectiveness of cetrimonium chloride can depend on the pH value of the final product. It is recommended that the pH be in a range compatible with cetrimonium chloride, typically between 4 and 7. The pH value can be adjusted by adding acids or bases as needed. For external use only.

EU safety information: In the European Union Cosmetics Regulation, cetrimonium chloride, cetrimonium bromide, and steartrimonium chloride are listed as alkyl (C12-C22) trimethyl ammonium bromide and chloride. These ingredients can be used as preservatives at a maximum concentration of 0.1%.

CIR (Cosmetic Ingredient Review) Expert Panel: The CIR Panel is an expert panel of a nonprofit organization established in 1976 to assess the safety of cosmetic ingredients used in personal care products. The CIR Panel consists of experts in toxicology, dermatology, pharmacology, and other relevant scientific disciplines. The panel independently reviews and evaluates scientific data on ingredients to determine if they are safe for use in cosmetics. The results and recommendations of the CIR Panel are published in the CIR Annual Scientific Review, which is available to the public and the industry and serves as a guide for cosmetic manufacturers regarding the safety of ingredients used in their products.

The safety of cetrimonium chloride, cetrimonium bromide, and steartrimonium chloride in cosmetic products was assessed by the CIR Expert Panel in 2012. After evaluating the available scientific data, the Expert Panel concluded that all three ingredients are safe for use in rinse-off cosmetic products at concentrations up to 10%, as well as for use in leave-on products at concentrations up to 0.25%. It is important to note that while these ingredients are generally safe, they can cause skin and eye irritation in some users, so it is advisable to conduct patch tests on a small area of skin before full use of the product.

Application: Hair conditioners, shampoos, hair masks, and styling products.

Source of raw materials: N-hexadecylamine and methyl chloride

Production method: Cetrimonium chloride is produced by the reaction of n-hexadecylamine with methyl chloride in the presence of sodium hydroxide.

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Animal testing: Not tested on animals

GMO: Non-GMO

Vegan: Contains no animal-derived components