



# INCROQUAT™ BEHENYL TMS-50

**INCI: Behentrimonium Methosulfate (and) Cetyl Alcohol (and) Butylene Glycol**

## Just the Right Touch

INCROQUAT BEHENYL TMS-50\* is a pastillated 50% active Behenyl (C22) quaternary conditioning agent and cationic emulsifier based on patented chemistry that enables the product to be supplied volatile-free and at the highest possible activity. As a higher active version of our original C22 quat INCROQUAT BEHENYL TMS (*INCI: Behentrimonium Methosulfate (and) Cetearyl Alcohol*), INCROQUAT BEHENYL TMS-50 contains less fatty alcohol and offers 'adjustable conditioning', a distinct benefit that allows formulators to manipulate the quat:fatty alcohol ratio and customize their product's conditioning performance. In skin care products it creates dense emulsions that spread easily and leave the skin feeling soft.

### Features / Benefits

- Non-volatile
- High activity
- 'Adjustable Conditioning'
- Substantive to skin and hair
- Excellent detangling/wet combing
- Exceptionally mild, non-irritating
- Safe for leave-on skin care
- Forms Elegant Cationic Emulsions
- Emulsifies Silicone
- Soft, Powdery Skin Feel
- Easy-to-use pastilles
- Economical 'value-in-use'

### Applications

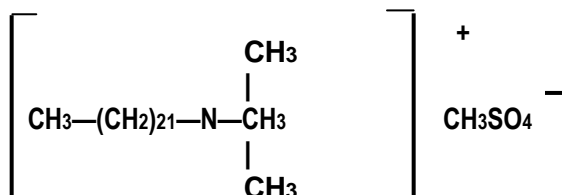
- Leave-on Conditioners
- Rinse-off Conditioners
- Detanglers
- Hair Relaxers/Straighteners
- Hair Dyes
- Creams & Lotions
- Silicone emulsions
- Shaving Products

INCROQUAT BEHENYL TMS-50 is supplied in a fatty alcohol/glycol solvent, making it safer and more environmentally friendly than other analogs that are traditionally supplied in Isopropyl Alcohol (IPA). As such, the product contains no volatile solvents, is non-hazardous and easier to handle. With the highest possible activity as a pastille, INCROQUAT BEHENYL TMS-50 has a lower fatty alcohol content that can be adjusted to suit, giving formulators the flexibility to create products that are custom-designed to target specific types of conditioning needs.

As a C22 methosulfate quat, INCROQUAT BEHENYL TMS-50 is a tremendously effective detangler for hair, yet is safe and gentle enough for leave-on skin care. It produces elegant cationic emulsions that are exceptionally mild and substantive to hair and skin. These emulsions leave hair tangle-free and feeling silky smooth and provide skin with a soft, powdery, and persistent after-feel.

*\*INCROQUAT BEHENYL TMS-50 and its use in personal care is covered under U.S. Patent 6,607,715.*

Chemically, INCROQUAT BEHENYL TMS-50 is a quaternary ammonium salt derived from the natural plant oil Colza, more commonly known as Rapeseed Oil, and is available in the methosulfate form of quat supplied in Cetyl Alcohol/Butylene Glycol. (See structure below.) The advantages that INCROQUAT BEHENYL TMS-50 offers in terms of lower irritation, more conditioning, better thickening, enhanced skin feel and improved stick structure, are a direct result of this composition.



**Figure 1: Behenyl Methosulfate Quat**

Croda's patented chemistry contributes to the unique features of INCROQUAT BEHENYL TMS-50. The precise combination of hydrophobicity and quaternary in the structure enhances deposition on the hair and promotes overall emulsion stability.

As a primary emulsifier and conditioning agent, INCROQUAT BEHENYL TMS-50 has a wide range of applications in hair care and skin care. Because of its exceptionally mild properties, it is an ideal choice for leave-on conditioners and leave-on skin care. It provides softening and emollient effects and gives body and thickness to emulsion systems.

#### **Quaternary Ammonium Compounds and How They Work**

Quaternary ammonium compounds are the primary and most frequently used conditioning agent in hair care. Their great popularity is due to the lubricity and static control they provide and to the conditioning benefits they offer in terms of detangling, combability and feel. The desirable conditioning properties of quats are largely the result of the substantive behavior of these compounds.

Substantivity is an adsorption phenomenon by which materials that have opposing charges or like compositions to a substrate are more readily adsorbed onto or attracted to its surface, and once there, are resistant to subsequent rinse-off. Chemically, quaternaries are a class of materials that contain at least one tetrasubstituted nitrogen, meaning they always carry a positive charge and are cationic regardless of pH. Adsorption tends to increase with an increase in the charge density of the quat at higher pH (>6.0). The complex protein of the hair fiber also contains chemical groups that are electrostatically charged. The surface of healthy virgin hair is neutral at pH 3.7 (IEP) and has a negative charge above this pH. Damaged or chemically treated hair has more negative sites. This increase in negative charge is primarily due to an increase in cysteic acid in the hair fiber. (Cysteic acid is a derivative of cysteine and forms when disulfide bonds are broken and not completely reformed as such.) Given that they have opposing charges, quaternaries are strongly attracted to the negative sites on the protein and are inherently substantive to hair. This same phenomenon leads to enhanced substantivity on the skin, as the skin is also negatively charged. Similarly to their behaviour on the hair, quaternaries are also resistant to wash off from the skin, so they confer a long lasting conditioned feel.

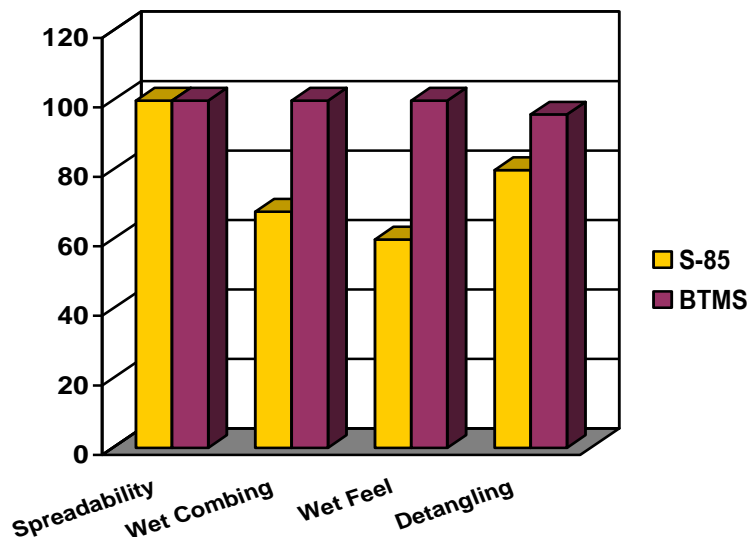
The enhanced feel properties of quats are due to the presence of fatty alkyl groups on the cation. The positively charged cation makes the whole molecule substantive in that the attached fatty chain also adsorbs onto the hair surface. This occurs because the formed quat micelles adsorbed at the hair surface solubilize the fatty alcohol. It is this fatty moiety and its hydrophobic properties that account for the high lubricity quats confer and the associated improvements in detangling and combability. While on the skin, this fatty moiety lends moisturization and softness.

Static electricity is the primary cause of flyaway and often occurs with combing. Repeated contact and subsequent separation of hair and comb during the act of combing generates positive charges causing them to accumulate on the hair. The occurrence of flyaway depends on three factors: the magnitude of the positive charge, its mobility and rate of dissipation from the hair fibers, and the distribution of the charge along the length of the combed hair fibers.

Quaternary compounds are known to reduce the incidence and/or severity of flyaway. First, they provide lubricating action that reduces the combing forces (friction and tangling) between the dry hair fibers and the comb, thus lessening the magnitude of the positive charge on the surface of the combed hair fibers. Secondly, they increase the surface conductivity of the hair. This causes the rate of charge dissipation from the hair fibers to be much faster, resulting in less of a net generated charge on the surface. Lastly, quaternaries allow for better moisture retention. When the water content at the hair surface is increased, there is a corresponding increase in surface conductivity. With less charge density and higher conductivity at the hair surface, flyaway is eliminated and the hair lies smooth again.

**Hair Care**

Due to the long chain of INCROQUAT BEHENYL TMS-50, the product is more hydrophobic in nature than conventional quaternaries. This results in better deposition of both quat and lipid on the hair surface. This hydrophobic driven adsorption can be enhanced by increasing the ratio of fatty alcohol to quat in the actual formula. The hydrophobicity and deposition behavior of INCROQUAT BEHENYL TMS-50 gives the product excellent wet combing properties, yet allows it to condition without the build-up associated with many polymeric quats. The bar chart below depicts the results of salon trials comparing the conditioning effects of behenyl quats to those of Stearalkonium Chloride.

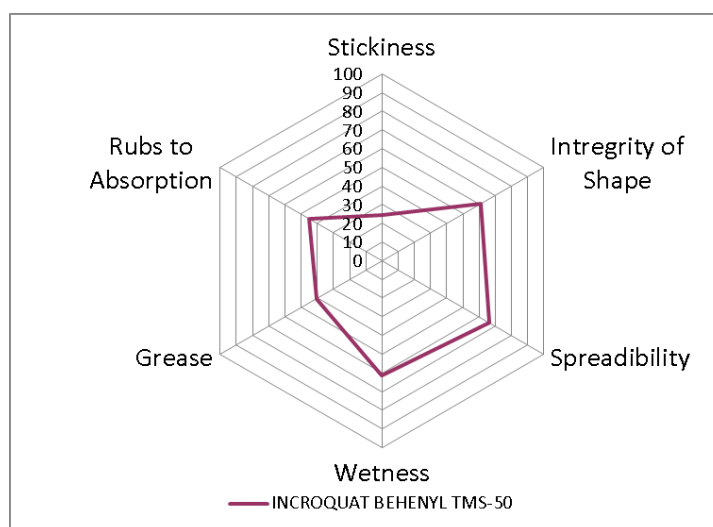


**Figure 2: Behenyl quats are known for their outstanding detangling and wet combing properties, as evidenced by the salon trial results.**

INCROQUAT BEHENYL TMS-50 is recommended for detanglers, cream rinses, and all types of conditioners. Besides wet combing, the product also gives hair excellent body and spring and reduces flyaway. INCROQUAT BEHENYL TMS-50 is also effective as a conditioner for ethnic hair care, especially in relaxer systems where it provides a soft feel and improved sheen.

### Skin Care

INCROQUAT BEHENYL TMS-50 forms elegant cationic emulsions, allowing formulators to produce skin creams and lotions create a unique initial sensory, leaving a soft, powdery after-feel that resists rinse-off. Sensory Spectrum Inc. (New Providence, NJ) uses a trained sensory panel in their Spectrum Descriptive Analysis (SDA) to evaluate up to 33 different sensory attributes and assigns quantitative measurement values to them. Six of the SDA attributes that make-up the initial sensory profile of for INCROQUAT BEHENYL TMS-50 are shown in Figure 3. All results are statistically significant.



**Figure 3: Initial Sensory Profile of INCROQUAT BEHENYL TMS-50**

INCROQUAT BEHENYL TMS-50 is a perfect choice for emulsifying silicone, an ingredient that is normally difficult to emulsify. Perhaps most important, though, is the fact that INCROQUAT BEHENYL TMS-50, when used to stabilize a cationic emulsion, is capable of mitigating any potential skin irritation. This discovery was made as a result of laboratory and salon testing.

The use of quaternary ammonium compounds in skin care products is relatively new. Given this fact, Croda commissioned a two part, double-blind independent clinical study to evaluate the irritancy and skin care properties of a selection of quats, as delivered from a prototype lotion at 1% active. Behenyl methosulfate quats were found to have a long-lasting *moisturizing effect* on the skin *in-vivo* and to be *non-irritating*, both *in vitro* and *in vivo*. We believe such a virtual lack of irritation may be due to the much lower Critical Micelle Concentration (CMC) that is unique to the Methosulfate form of the Behenyl quat. This low CMC means that there is very little of the monomer present in the quat. It is in the monomeric form that the surfactant is more likely to penetrate into human tissue and become a source of irritation.

The study consisted of an *in-vitro* bioassay for cytotoxicity using a MatTek Epiderm Skin Model and a 15-day *in-vivo* clinical trial evaluating the effects of quats on irritancy, moisturization and barrier skin function. Testing also determined that skin treated with Behenyl methosulfate quats do not experience barrier dysfunction (unaffected TEWL scores) and resist insult by ALS. (Please refer to DS-122.doc for full information)

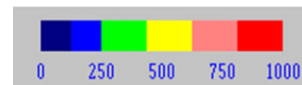
To further support these findings, an additional study was also conducted. Using Laser Doppler Blood Flow Imaging, the irritation potential of the INCROQUAT BEHENYL TMS-50 was tested versus Cetrimonium Chloride and Dimethyldioctadecylammonium Chloride (Varisoft® TA-100, Goldschmidt), in water and as part of a simple cationic emulsion. 1% Sodium Lauryl Sulfate in water was used as a positive control. The test was performed on 10 subjects. The Laser Doppler results were substantiated by visual grading of both erythema and dryness.

**Laser Doppler Results-**

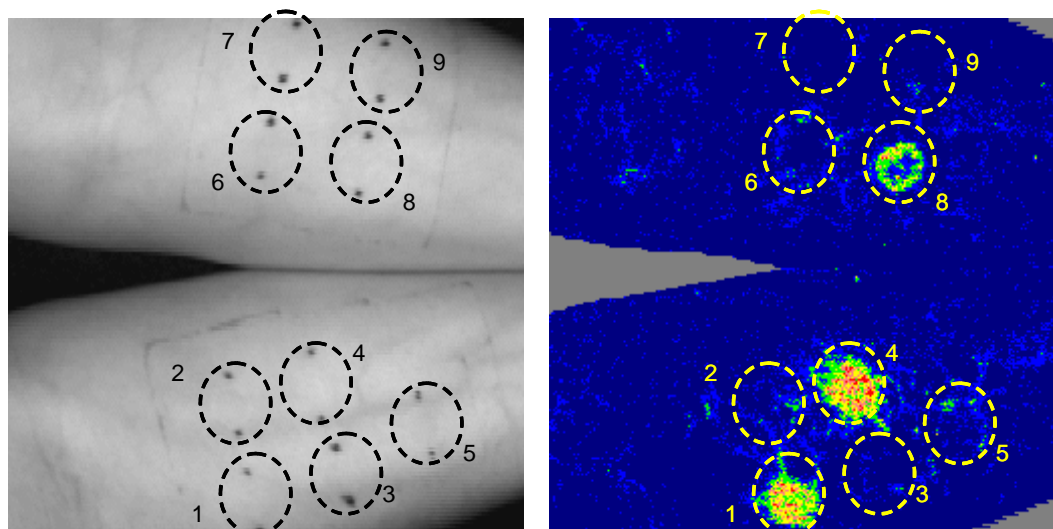
Site No.	Test Product	Mean Value – Blood Flow (Perfusion Units)
1	Cetrimonium chloride in water	320.6
2	INCROQUAT BEHENYL TMS-50 in water	99.9
3	Varisoft TA-100 in water	86.7
4	1% Sodium Lauryl Sulfate in water	514.2
5	Distilled Deionized Water (DDW)	106.7
6	Varisoft TA-100 emulsion	86.0
7	INCROQUAT BEHENYL TMS-50 emulsion	69.5
8	Cetrimonium chloride emulsion	167.7
9	Nonionic emulsion	78.7

**Table 1: INCROQUAT BEHENYL TMS-50 emulsions are exceptionally mild on skin**

**Blood Flow by Laser Doppler Imager (Perfusion Units)**



09 KMR



**Figure 4: Laser Doppler Images of Blood Flow. The increased blood flow, typical of irritation, is clearly seen at Sites 1, 4 and 8. (Cetrimonium Chloride in water, 1% SLS in water and the Cetrimonium Chloride emulsion)**

Erythema and Dryness Scores – Erythema and dryness of the treatment sites were graded on the following scale:

0	=	None
1	=	Slight
2	=	Moderate
3	=	Severe

**Erythema and Dryness results**

Site No.	Product Name	Erythema	Dryness
1	Cetrimonium chloride in water	2.20	1.50
2	INCROQUAT BEHENYL TMS-50 in water	0.00	0.00
3	Varisoft TA-100 in water	0.20	0.00
4	1% Sodium Lauryl Sulfate in water	2.70	0.50
5	Distilled Deionized Water (DDW)	0.10	0.00
6	Varisoft TA-100 emulsion	0.00	0.10
7	INCROQUAT BEHENYL TMS-50 emulsion	0.00	0.00
8	Cetrimonium chloride emulsion	1.40	0.80
9	Nonionic emulsion	0.00	0.10

**Table 2: INCROQUAT BEHENYL TMS-50 creates no erythema or skin dryness**

As a result of Laser Doppler Blood Flow measurements, the three most irritating products were found to be 1% SLS in water (Site 4), Cetrimonium Chloride in water (Site 1) and the Cetrimonium Chloride emulsion (Site 8) with mean blood flux (PU) values of  $514.2 \pm 152.1$ ,  $320.6 \pm 180.5$  and  $167.7 \pm 106.2$  respectively. All the other products showed values under 100 perfusion units.

The least irritated site was Site 7, INCROQUAT BEHENYL TMS-50 emulsion, with the blood flux value of  $69.5 \pm 15.6$  perfusion units.

The visual grading of erythema showed results similar to the blood flux measurements. The mean values exposed the three most irritating products as: 1% SLS in water (Site 4), Cetrimonium Chloride in water (Site 1) and the Cetrimonium Chloride emulsion (Site 8) with mean grades of  $2.70 \pm 0.48$ ,  $2.20 \pm 0.79$  and  $1.40 \pm 0.84$  respectively. The mean grades for other product sites were either 0.2 or less.

The dryness grades showed the most dryness present at Site 1, followed by Site 8 and then Site 4.

**CONCLUSION**

INCROQUAT BEHENYL TMS-50 offers formulators tremendous benefits as a high actives behenyl quat. First of all, the product represents patented chemistry which means a real point of difference. Secondly, INCROQUAT BEHENYL TMS-50 provides 'adjustable conditioning', giving you solutions for today's more targeted hair care products. Thirdly, INCROQUAT BEHENYL TMS-50 is soft and gentle on the skin, letting you create creams and lotions that are substantive and have great feel characteristics. What's more, INCROQUAT BEHENYL TMS-50 is vegetable-derived, pastillated and solvent-free for easy, safer handling. Lastly, INCROQUAT BEHENYL TMS-50 gives formulators a cost effective means of creating customized conditioners or leave-on skin care products.

Recommended use levels are 1 - 10%.

**Table 3: Typical Analysis**

Appearance	Pastille
Color	White to off-white
Odor	Characteristic
pH (2% aqueous)	5.0-7.0
% actives (MW=504.4)	48.0-51.0

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**Without a Trace Make-Up Remover****SC-593**

See and feel the difference of this silky smooth make-up remover with CRODAMOL™ SFX. This INCROQUAT™ TMS-50 emulsion formula removes make-up effectively, in as little as 30 seconds! CRODAMOL SFX's unique chemistry gives it the power to easily solublize hard to remove lipstick, mascara and eye-liner without leaving a trace.

<b>Ingredients</b>	<b>%</b>
<b>Part A</b>	
Deionized Water	63.00
Propylene Glycol	5.00
<b>Part B</b>	
CRODAMOL SFX (PPG-3 Benzyl Ether Myristate)	25.00
INCROQUAT TMS-50 (Behentrimonium Methosulfate (and) Cetyl Alcohol (and) Butylene Glycol)	4.00
CRODACOL™ C-70 (Cetyl Alcohol)	2.00
<b>Part C</b>	
Propylene Glycol and Diazolidinyl Urea (and) Propyl Paraben (and) Methyl Paraben <sup>2</sup>	1.00

Suppliers: **1. CRODA** 2. Germaben II, Ashland

Viscosity- 42,000 cPs (Brookfield RVT Spindle TC @ 10 rpm, at Room Temperature)

pH: 5.50

**Procedure**

Combine Part A and Part B ingredients separately with mixing and heat each to 80°C. Remove heat and continue mixing, maintaining temperature at 80C for 10 minutes. Remove heat and continue mixing until batch cools to 40C. Add Part C and cool to room temperature. Adjust pH to 5.50 with TEA.

Ref. 2060-089-2

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**Replenish and Strengthen Leave-in Conditioner with CUTISSENTIAL™ 18-MEA 40****HP-356**

This light leave-in conditioner is designed to revitalise the hair. CUTISSENTIAL 18-MEA 40 replenishes the lipid layer and restores the hairs' natural hydrophobicity, while the dual action KERAIVIS™ acts as both a cortex strengthening complex and cuticle reinforcer for anti-breakage benefits. INCROQUAT™ BEHENYL TMS-50 improves combing properties of the product and the HYDROTRITICUM™ PVP contributes to a moderate hold and soft feel. CRODAROM® ROCK CRYSTAL helps to fortify the hair against environmental damage.

<b>Ingredients</b>	<b>%</b>
<b>Part A</b>	
Water	84.20
Glycerin	5.00
<b>INCROQUAT BEHENYL TMS-50</b> (Behentrimonium Methosulfate (and) Cetyl Alcohol (and) Butylene Glycol)	1.50
<b>CUTISSENTIAL 18-MEA 40</b> (C10-40 Isoalkylamidopropylethyldimonium Ethosulfate (and) Dipropylene Glycol)	2.50
<b>CRODACOL™ 1618</b> (Cetearyl Alcohol)	1.50
<b>KERAIVIS</b> (Hydrolyzed Vegetable Protein PG-Propyl Silanetriol)	2.00
<b>HYDROTRITICUM PVP</b> (Hydrolyzed Wheat Protein /PVP Crosspolymer)	1.00
<b>CRODAROM ROCK CRYSTAL</b> (Water (and) Propylene Glycol (and) Quartz)	1.00
Water (and) Sodium Benzoate (and) Potassium Sorbate <sup>2</sup>	0.80
Fragrance <sup>3</sup>	0.50

Suppliers **1. Croda** 2. Euxyl K712, Schülke & Mayr 3. Tranquil Waters Fragrance 110M2, Flavor and Fragrance Specialties

pH: 5.5 ± 0.5; Viscosity: 2,000 cps ± 10% (RVT Spindle 5 @ 10 RPM, 25°C)

**Procedure**

Combine the deionized water, glycerin, CUTISSENTIAL 18-MEA-40 and INCROQUAT BEHENYL TMS-50 and heat to 65-70°C with mixing. Homogenize the batch (40 sec/100g of the product). Finally, add the HYDROTRITICUM PVP, KERAIVIS, CRODAROM ROCK CRYSTAL, preservative and the fragrance when the batch cools down to 40°C.

**Salon Evaluation**

The Replenish and Strengthen Leave-In Conditioner was tested in a whole head salon study involving five panellists. The study involved assigning performance ratings for key wet and dry attributes by a trained cosmetologist. A grading scale of 0.5 to 5 was used, with the following scale definitions:

**Scale**

5.0 = Excellent

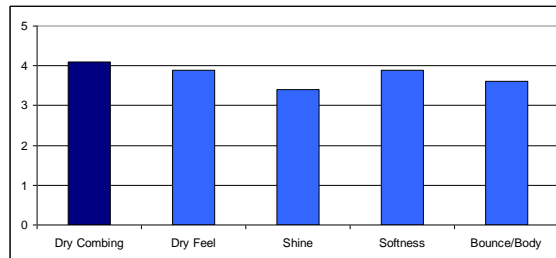
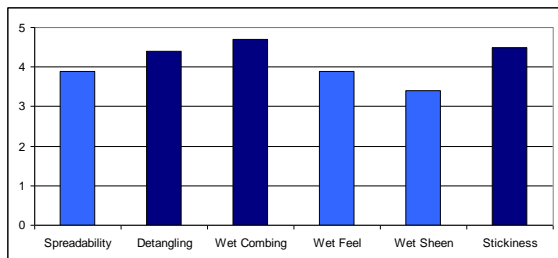
4.0 = Very Good

3.0 = Good

2.0 = Fair

1.0 = Poor

The salon evaluations detailed below show that the leave-in Replenish and Strengthen Conditioner has immediate perceivable aesthetic benefits in addition to its longer term replenishing and strengthening effects. The INCROQUAT BEHENYL TMS-50 and CUTISSENTIAL 18-MEA-40 combine to give very good to excellent combing properties while the non-sticky formulation also delivers good to very good properties in all remaining key attributes.



■ = Very Good to Excellent

■ = Good to Very Good

**References**

AB8-2-1

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