PERSONAL CARE

Crodamol STS

Superior to Silicone

Over the last decade, silicones and silicone derivatives have literally infiltrated all areas of the personal care market. Dimethicones have moved from antiperspirants into liquid makeup, sunscreens and lipsticks at significant use levels. In hair care, silicones have become the benchmarks to fulfil the promise of shiny, silky hair. Now, thanks to Croda technology, formulators have a multi-functional alternative in Crodamol STS.

Crodamol STS is an emollient ester based on patented Croda chemistry and offers many of the desirable attributes of silicone (dimethicone), especially in terms of shine and feel characteristics, plus a number of other benefits dimethicone does not provide.

Product	INCI name	Appearance	Molecular weight
Crodamol STS	PPG-3 Benzyl Ether Myristate	Clear pale yellow liquid	495

Features / benefits

- Superior to Silicone
- Excellent detackifier
- Higher refractive index (RI)
- Film-forming
- Wide compatibility
- Easily emulsified
- Yields very stable emulsions
- Good pigment wetting property
- Provides dry emolliency
- Reduces dry-off of essential oils
- Helps dissolve benzophenone-3
- Excellent water spreader
- Low skin migration
- Silicone-like feel and functionality
- Improves emulsion aesthetics
- Reduces greasiness of high SPF sunscreens
- Excellent wax solvency
- Lessens whitening effect of antiperspirant salts
- Good binder for pressed powders
- Shine/gloss enhancer for hair
- Foam stabiliser

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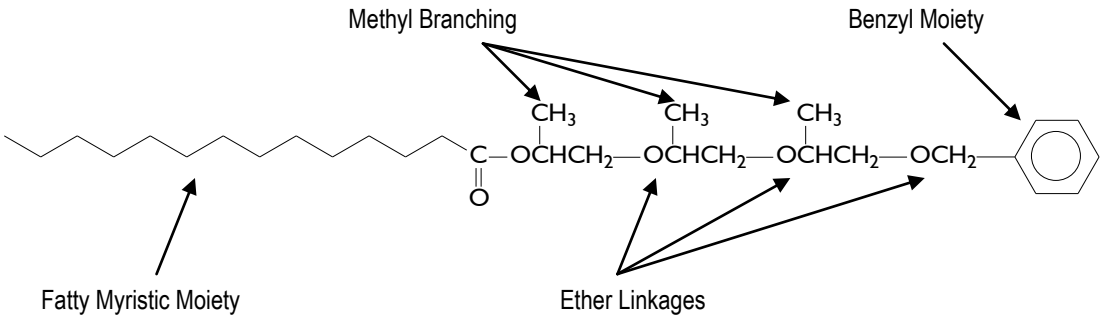
Structure of Crodamol STS



*Crodamol STS is and its use in personal care applications are covered under US Patent 6,987,195 and 7,217,424.

Structural attributes

- Alkoxylation improves dispersability and modifies feel
- Methyl branching promotes fluidity and modifies feel
- Ether linkages increase polarity, improve compatibility with pigments and modify feel
- Benzyl moiety confers better compatibility with sunscreens, sterols and fragrances

Applications

- Make-up
- Sunscreens
- Antiperspirant/deodorant sticks
- Lip care
- Creams and lotions
- Hair conditioners
- Shine products
- Styling aids
- Microemulsion gels
- Hydroalcoholic systems

'Superior to Silicone'

Silicones have enjoyed wide use in personal care products due to their exceptional feel characteristics and shine boosting properties. Given both its silicone-like feel and silicone-like benefits, Crodamol STS is ideal as either a complete or partial replacement for dimethicone, especially in cases when dimethicone might cause formulating or stability problems.

Emulsifying Advantages

As an ester, Crodamol STS is non-volatile and can enhance the stability of high silicone emulsions, which are typically difficult to emulsify. Crodamol STS will not flash off with alcohols in hydroalcoholic systems, and instead, leaves behind a desirable film for surface improvement. These films also reduce spreading, providing low skin migration, and help prevent dry-off of essential oils and fragrances.

Crodamol STS itself is easy to emulsify due to the presence of both polar and non-polar groups in its structure. Consequently, less emulsifier load is required resulting in a more energy efficient and economically friendly formulation. The stability of model dispersion systems was assessed via a Phase Separation Time experiment (PST) which compares aqueous solutions of Crodamol STS with those of C_{12-15} Alkyl Benzoate (an ester of similar chemical structure) and Dimethicone. The experiment demonstrated enhanced dispersability of Crodamol STS in water compared with the other test products (See figure 1).

Phase Separation Assessment

The increased polarity of Crodamol STS is responsible for its higher PST, resulting in more stable emulsions and dispersions, lower emulsifier requirements and less irritation potential.

Figure: 1a: Ester and silicone systems immediately after agitation (T = 0)

Figure: 1b: Ester and silicone systems 10 minutes after agitation (T = 10)

Functional Advantages

Reduction of Formula Tack

In skin care, AP/Deo and cleansing applications tack is extremely undesirable. Many emollients and occlusive film-formers are utilised within these systems for the functional attributes they confer related to skin conditioning. Through the careful selection of raw materials the associated tack can be minimised, or even removed. Crodamol STS not only confers excellent skin feel and lubricity, but is also able to reduce the tack associated with materials such as petrolatum, polyisobutene and some lanolin fractions; materials which are widely used in skin, colour cosmetic and body applications.

Tack Measurement – The Cotton Ball Test

The cotton ball test is a rudimentary, but highly visual, methodology for the assessment of tack. Quite simply the test relates the tack associated with a certain raw material to the quantity of cotton fibres removed from a cotton ball applied to a film of the test ingredient. Petrolatum, polyisobutene and lanolin were all assessed for tack against the same materials containing 20% Crodamol STS. Digital images of the test films are illustrated in figures 2a – 2c. Increasing quantities of adhered cotton fibres can be seen in the pure ingredients compared with those same ingredients with Crodamol STS, illustrating the detackifying power of this novel ester.

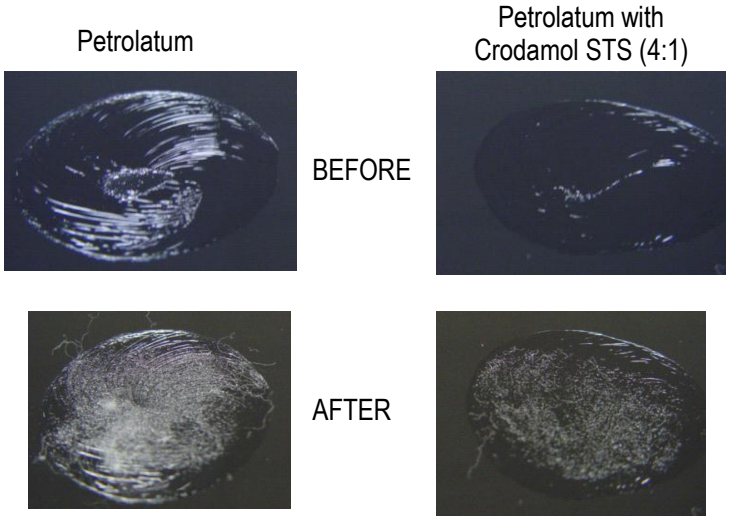


Figure 2a: The inclusion of 20% Crodamol STS reduces the tackiness of petrolatum

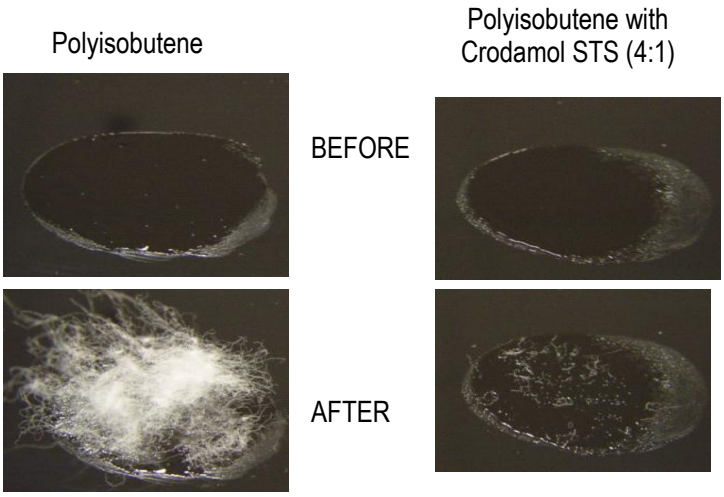


Figure 2b: The inclusion of 20% Crodamol STS reduces the tackiness of polyisobutene

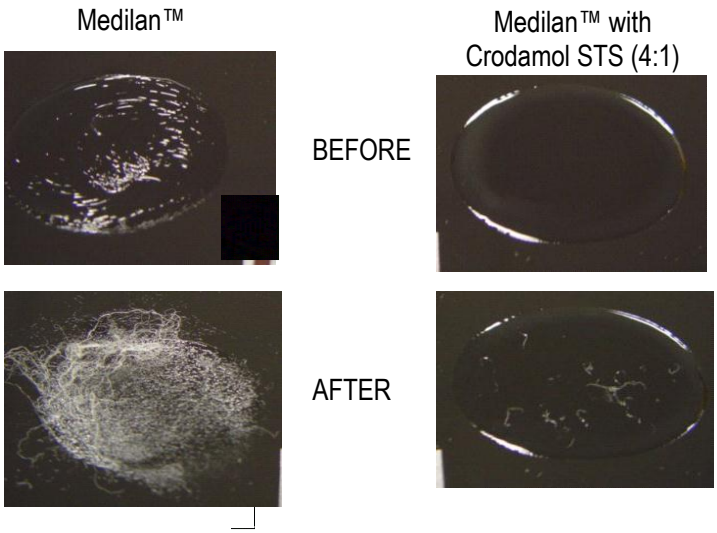


Figure 2c: The inclusion of 20% Crodamol STS reduces the tackiness of Medilan™

Formulating Advantages

Make-up

Unlike silicone, Crodamol STS is effective in wetting inorganic pigments (colour cosmetics and sunscreens alike). Although Crodamol STS has a relatively high neat viscosity (100 cps), its suspension viscosities in Mica, Titanium Dioxide and Zinc Oxide are only 11,860, 33,640, and 10,000 cps, respectively, the values of which all fall within the acceptable range for good pigment wetting.

In liquid foundation, Crodamol STS allows for ample application time, helps reduce whitening, and adds to the feel properties and slip of the product. An in-house sensory panel evaluating a Crodamol STS foundation formula (see Croda formula C5162) rated the following attributes as superior:

- Soft, smooth feel
- Uniform colour
- Good coverage
- Matt finish
- Easily spread and blended
- Comfortable to wear

Crodamol STS demonstrates good wax solvency, making it ideal in lip care applications. Sticks containing Crodamol STS are translucent and have a fine crystal structure and texture (Cloud Point: 67ºC; Pour Temperature: 72ºC). As Crodamol STS has a higher refractive index (RI) than the traditional silicones it is especially recommended for lip-gloss products (see Croda formula C5165) and 'wet look' lipsticks. With its slow spreading characteristics Crodamol STS also helps prevent the feathering and creeping that can occur with silicones.

Sunscreens

Like silicone, Crodamol STS helps reduce whitening in sunscreens but also helps to disperse physical sunscreens like Titanium Dioxide and Zinc Oxide, which silicones do not typically do. In addition, it forms thin uniform films that provide good playtime for more even spreading, as well as better wash-off resistance for higher SPFs. Silicones spread spontaneously on skin and are not used for this purpose whereas Crodamol

STS offers low skin migration. It can, also, solubilise Benzophenone-3 (Oxybenzone). Figure 3 demonstrates Crodamol STS's ability to solubilise 20% Benzophenone-3 as compared to Dimethicone 200 cst and a very commonly used ester, C_{12-15} Alkyl Benzoate.

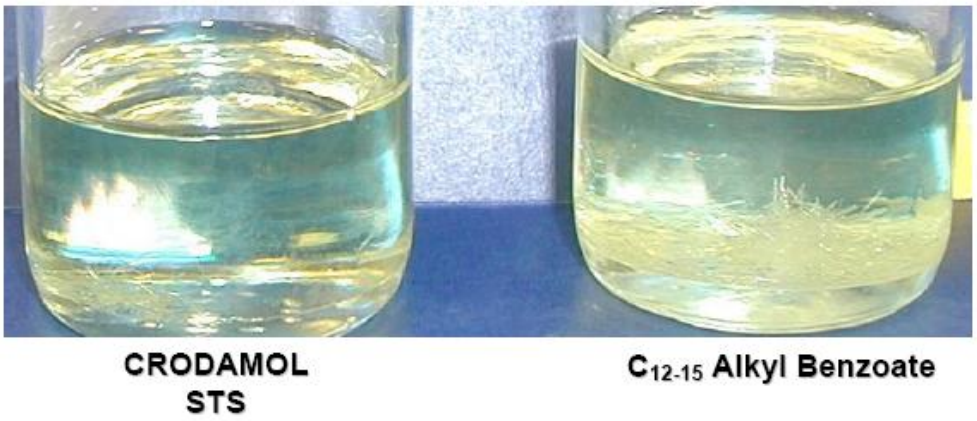


Figure 3: Crodamol STS solubilises Benzophenone-3 better than C_{12-15} Alkyl Benzoate

As can be seen, the solubility of B-3 in CRODAMOL STS, far exceeds that of C_{12-15} Alkyl Benzoate. In Dimethicone 200 cst, the Benzophenone-3 completely crystallised out upon cooling.

Antiperspirant Systems

Crodamol STS enhances the after feel of anti-perspirant and deodorant systems, as well as reducing tack and improving the glide of stick formulations (see Croda formula C5169). Crodamol STS is a very effective wetting agent for antiperspirant actives and reduces the whitening effect of fatty alcohols to provide non-whitening formulations. As formulation clarity is an additional benefit of high RI esters, Crodamol STS allows the production of clear suspensions.

Reduced Whitening from Antiperspirants

To demonstrate the reduction of AP whitening, three classic style stick formulations were made: a control, a 100% replacement of isosorbide laurate with Crodamol STS, and a 50% replacement of isosorbide laurate with Crodamol STS.

The stick formulations were applied to draw downs to demonstrate the whitening effect, or lack there of, of the products. On the following page are the formulations and draw down images.

	Control %w/w	CRODAMOL STS %w/w	CRODADMOL STS & Isosorbide Laurate %w/w
Cyclomethicone (D4/D5)	45.0	45.0	45.0
Crodamol STS	**-----**	**10.0**	**5.0**
Isosorbide Laurate	10.0	-----	5.0
Stearyl Alcohol	20.0	20.0	20.0
Hydrogenated Castor Oil	5.0	5.0	5.0
Aluminum Salt	20.0	20.0	20.0

Table 1: Formulation for testing reduction of whitening in AP sticks.

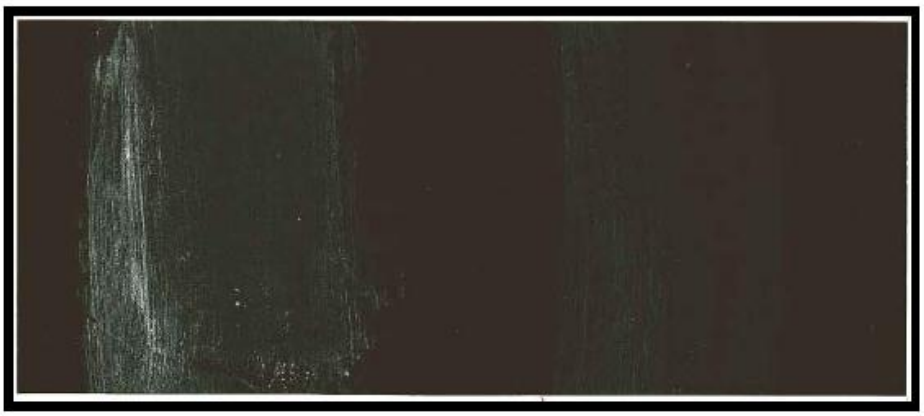


Figure 4: 100% replacement of isosorbide laurate with Crodamol STS in a test stick AP formulations yields significantly less whitening.

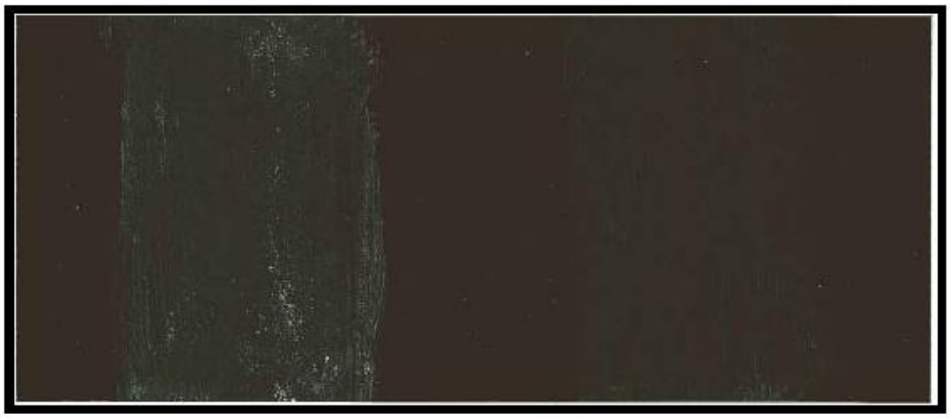


Figure 5: 50% replacement of isosorbide laurate with Crodamol STS in a test stick AP formulations yields significantly less whitening.

Emollient Skin Spreading Factor (ESSF)

Croda's Emollient Skin Spreading Factor is a predictor of an emollient's spreading behaviour and is a figure that represents the ratio of the final area of coverage divided by the initial area over which the emollient was applied. (Refer to Emollient Skin Spreading Factor DS128.) With an ESSF of 3.97, Crodamol STS spreads quite slowly and forms relatively stationary, cohesive films. Most silicones, in contrast, spread spontaneously on the skin. This kind of spreading behaviour is not always desirable, as it can cause adverse effects, such as creeping in make-up or migration of actives in sunscreens. Crodamol STS can actually improve the spreading behaviour of dimethicones, and is more effective than these materials in systems that contain pigments or those in which efficacy depends on a certain type of spreading.

The skin spreading behaviour of emollients depends on several factors—molecular weight, chemical structure, viscosity and fatty character. High molecular weight esters, particularly those with long straight-chain structures, are usually quite viscous and spread slowly. In contrast, branched chain emollients tend to be more

fluid and spread quickly on the skin. Fatty character affects spreadability in terms of its sensory aspects perceived from the action of rubbing. With quick spreading emollients, there appears to be an instantaneous sensation of high lubricity that subsides quickly. With slower-spreading emollients, the sensation of lubricity is more subtle but the effect is more long lasting.

Water Spreadability

Though Crodamol STS offers low migration on the skin, it offers excellent spreading on the surface of water. Crodamol STS was compared to mineral oil to determine the spreading capabilities on water's surface. Talc, which was used as a visual, was sprinkled on the surface of a pan of water. Drops of Crodamol STS and mineral oil were then placed in the centre of the talc covered pan to note any movement.

Figure 6: The spreadability of Crodamol STS on the surface water, using talc as a visual indicator

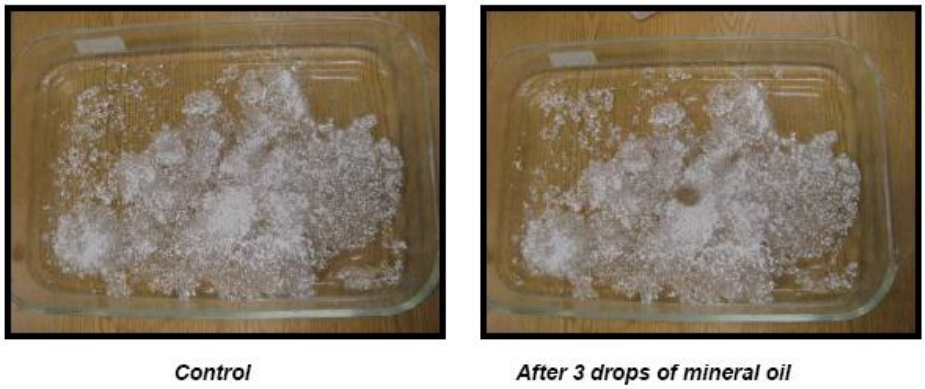


Figure 7: The spreadability of mineral oil on the surface of water, using talc as a visual indicator

Figures 6 and 7 clearly show that the ability of Crodamol STS to move across the surface of water is far superior to that of mineral oil as indicated by the movement of the talc.

This makes Crodamol STS ideal for use as the primary emollient in bath oils, after shower body sprays and body oils, without the need for an additional spreading agent within the formulation.

Refractive Index and Shine Enhancement

In terms of hair care, one of the major attributes associated with silicone is shine.

Crodamol STS has been shown equivalent, and in some ways superior to silicone in providing shine. Cyclomethicone, and occasionally, a combination of cyclomethicone and dimethicone, have been widely used

for improving sheen. Sheen formulas typically contain 60-90% oils/silicone and a solvent carrier such as alcohol.

All materials reflect and refract light (alter its angle). When light passes from one medium to another, its path is bent. The refractive index is a ratio that reflects this and can be defined as the speed of light in vacuum over the speed of light in material. The refractive index of light in vacuum is one. Since light slows down when it enters a substance, the refractive index of any material will always be greater than one. The higher the refractive index is, the smaller the refractive angle of light is, and hence, the higher the light flux (intensity) that is reflected from the surface.

Measuring the refractive index of a material is an indirect, but reliable method of predicting shine potential. This theory holds true for Crodamol STS**,** which has a refractive index of 1.4696. Cyclomethicones and dimethicones both have lower refractive indices, ranging from 1.394-1.398 and 1.375-1.403, respectively. With its higher refractive index, Crodamol STS would be expected to give more shine than silicone alone.

Figure 8: Crodamol STS visibly enhances shine. In the tress treated with Crodamol STS enhanced shine is that area where hair colour looks richer and the is more intense (indicated by the arrow)

In accordance with the above approach a colour image analysis method was used to determine hair shine. Using this method, hair tresses treated with a commercial shine product control and with 2% Crodamol STS added to create the test system were placed in a black, glare-free 'shine box' with a uniform light luminance (~1600 lux). Digital images of the hair samples were taken with a Sony DSC-F707 digital camera set at the highest resolution. Image Pro Plus 4.5 software was then used to measure the intensity of red, green and blue light on the hair surface. The Luster Index[1] (L) is a value that reflects the degree of hair shine and is defined as the ratio of the blue light intensity of the highlighted portion (BH) of the hair to the red light intensity of the adjacent dark portion (RD) of the hair: L = BH/RD. The Luster index of hair treated with the commercial shine product containing Crodamol STS was 10.0, compared to 8.32 for hair treated with the commercial product alone. These values correlated with the directional trend in the solution refractive indices of the Crodamol STS product (RI=1.413), compared to the retail product alone (R=1.403).

Besides lustre, a high refractive index promotes clarity, giving Crodamol STS additional use in other applications:

- Ideal for clear antiperspirants/deodorants and microemulsion gels
- Remains clear in hydroalcoholic systems
- Works synergistically with cyclomethicone to improve sheen in hydroalcoholic styling aids
- Improves wet sheen in conditioners as total or partial replacement for silicone

Hair Shine Imaging System

Croda is utilising a new system to evaluate shine in hair. This equipment provides more objective quantification of shine and can be used to calculate the luster index for all shades of hair (natural or dyed). The luster index (L) is calculated using the following equation:

$$L = (S-D)/D$$

Where;

S = the area underneath the specular curve

D= the area underneath the diffuse curve.

The specular profile is created by the amount of light that is reflected from the hair surface. The diffuse profile is created by the amount of light that is scattered from the hair surface. According to the equation, the more light that is reflected (i.e. the higher the specular curve) and the less light that is scattered (i.e. the lower the diffuse curve) provides a higher luster index (i.e. more shine).

Several different hair colours and types were evaluated in order to demonstrate their varying luster values (see table 2 below). All hair tresses were treated with HP-254 Shine Boosting Spray containing 45% **CRODAMOL STS** and 55% Cyclomethicone. After treatment of each tress with the Shine Boosting Spray, each tress was analysed by the Hair Shine Imaging System. The higher the L value, the more shine.

Table 2: Hair samples used for shine analysis with Hair Shine Imaging System and their corresponding luster values

Hair Type	Corresponding Code	Luster Value
Medium Brown Hair	MB	6.41
Light Bleached Hair	LB	0.43
Dark Bleached Hair	DB	1.21
Oriental Black Hair	OB	9.80
Dyed Light Bleached Hair (Dye: Medium Auburn hair Colour)	CLB	3.63
Dyed Dark Bleached Hair (Dye: Medium Auburn hair Colour)	CDB	4.06

In order to demonstrate the capabilities of the Hair Shine Imaging System, black, light bleached and brown hair was measured for shine and then again after treatment with the Shine Booster formulation containing Crodamol STS. Figure 9 shows the increase the in luster reported by Hair Shine Imaging System for the hair treated with Crodamol STS.

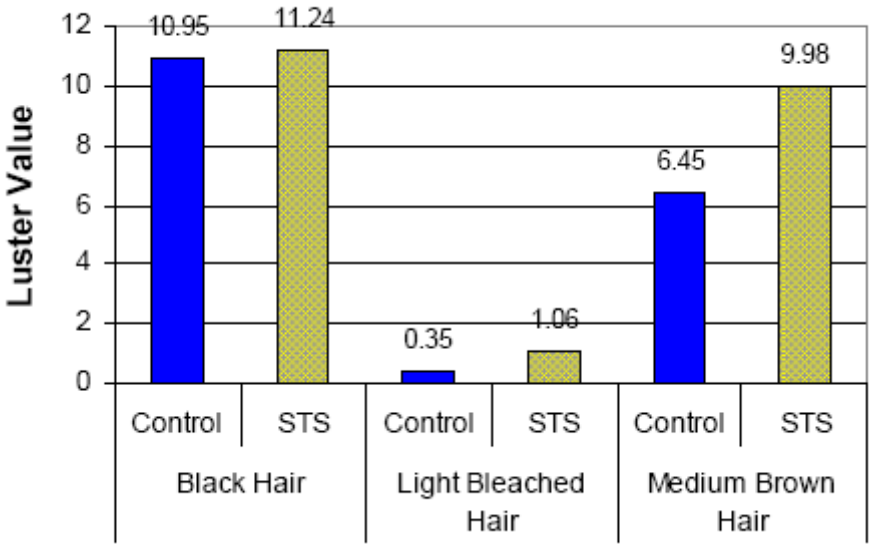


Figure 9: Treating tresses with the Shine Booster formulation increases the luster reported by the Hair Shine Imaging System

Polarised images visually demonstrate the difference in diffusion of shine between the control and Crodamol STS formulation. The less diffusion and more reflectance, results in a greater luster value. (This is demonstrated in figures 10 and 11.)

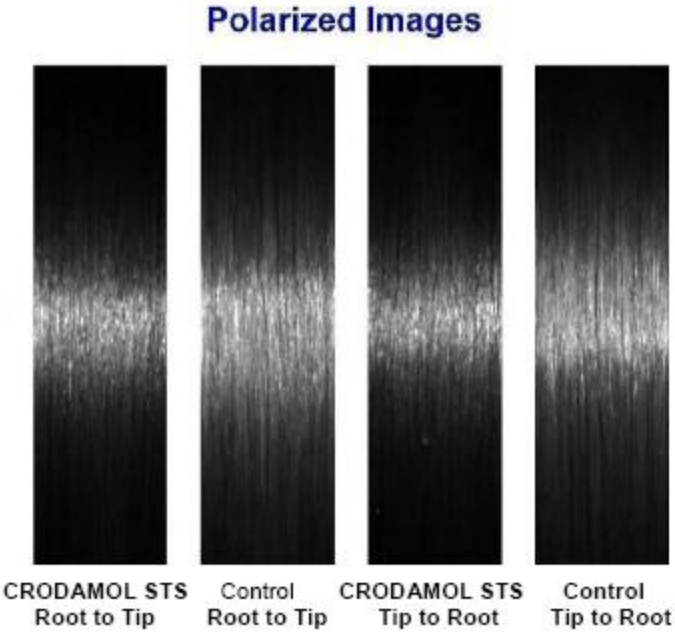


Figure: **10 The comparison between the control and the hair tress (light bleached hair) treated with Crodamol STS indicates that the tress that is treated has less diffusion and more reflectance, resulting in a larger luster value**

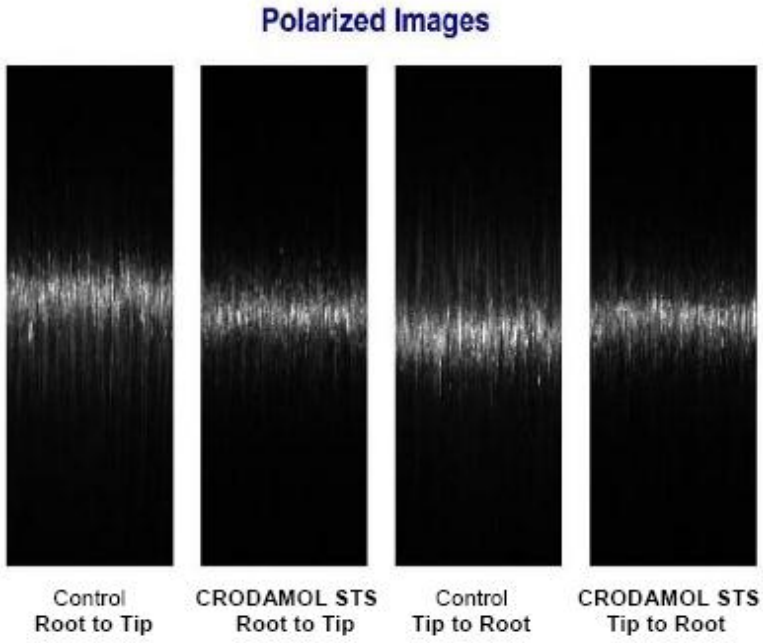


Figure 11: The comparison between the control and the hair tress (medium brown hair) treated with Crodamol STS indicates that the tress that is treated has less diffusion and more reflectance, resulting in a larger luster value

Measuring Cuticle Smoothness

Using the Hair Shine Imaging System, the surface smoothness of the hair can also be measured, as the smoothness of the hair is directly related to the shine. To measure surface smoothness, the luster of the hair is calculated by looking at the specular profile of the hair in two different orientations: root to tip and tip to root.

To measure the smoothness of the hair, or the cuticle angle difference, the following calculation is utilised:

$$\theta = 2\alpha$$

Where α = the cuticle angle and θ = the difference of angle between the two peaks of the specular profiles (Root-to-Tip angle measurement) – (Tip-to-Root angle measurement). The smaller the α value, the smoother the hair cuticle surface.

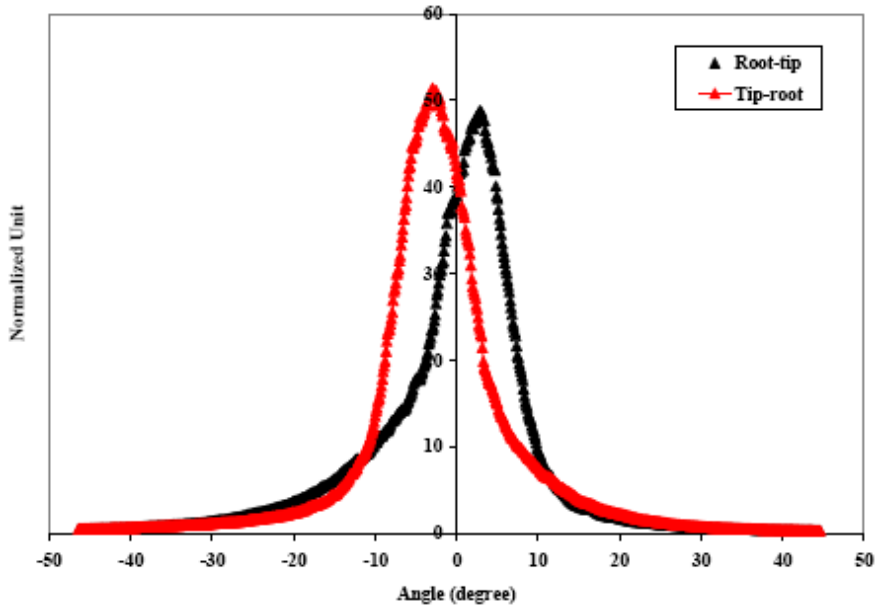


Figure 12: Typical reflection profiles from a hair fibre in the Root-to-Tip and Tip-to-Root orientations

In all hair types tested, the application of the Shine Boosting Spray containing the Crodamol STS smoothes the hair cuticle (figure 13).

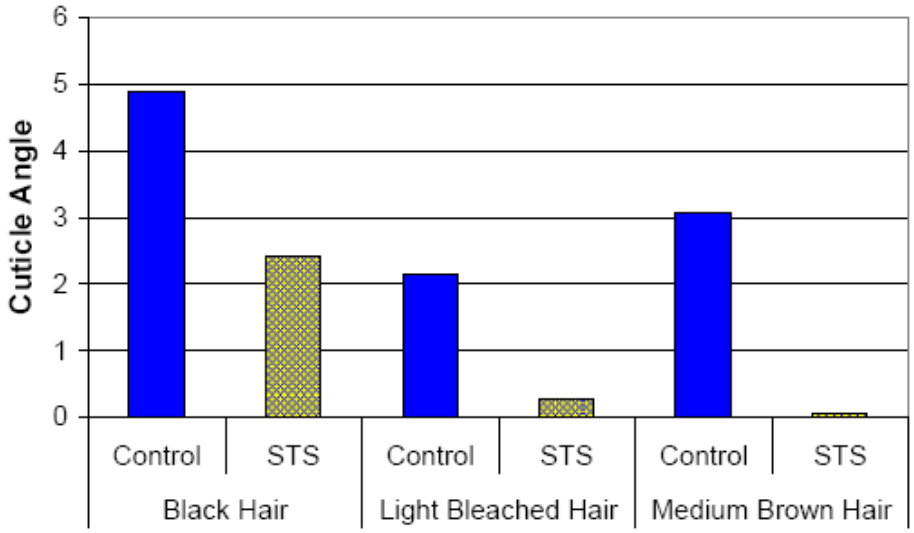


Figure 13: The cuticle angles of the different hair types decrease dramatically after treatment with Crodamol STS

Hair Conditioning and Detangling

As well as improvement of hair gloss, another well known function of silicones is their ability to improve the lubricity of hair resulting in better conditioning performance. The conditioning attributes of Crodamol STS have been assessed in two ways. Firstly, a Crodamol STS conditioner was compared against a control conditioner from a standard rinse-off hair conditioner control; and secondly a direct assessment of Crodamol STS versus an amidosilicone fluid was performed from an intensive conditioner system.

The creation of a laboratory prototype rinse –off conditioner containing a quantity of cationic quaternary ammonium compound and fatty alcohol allowed the benefits of Crodamol STS on combing (peak force and total work), contact angle (surface lipophilic character) and shine improvement on hair fibres to be assessed.

The formulation utilised for this assessment is detailed below:

Part A	
Crodazosoft DBQ	2.23%
Crodacol S70	2.00%
Crodacol C70	0.50%
Super Sterol Ester	1.00%
Crodamol STS	4.50%
Crodacel QM	0.20%
Deionised water	85.27%

Part B	
Crosilk 10,000	1.00%
Hydrotriticum 2000	1.00%
Keravis	1.00%
Phytexcel Green Tea	0.10%
Phytexcel Chamomile	0.10%
Phytexcel Sea Buckthorn	0.10%

Part C	
Phenova	1.00%

Viscosity = 11,200cps with STS, 16,000 cps w/o STS; pH = 4.5

Control conditioner was as above but without Crodamol STS.

This addition of Crodamol STS in this formulation can be expected to positively affect the combing properties of hair due to the enhanced lubricity at the fibre surface. Comparative assessment of the control conditioner against the test conditioner with Crodamol STS demonstrated this to be true. In both bleached and virgin hair tresses the combing forces were seen to be reduced, but the effect was most markedly noted from assessment of virgin hair fibres where the inclusion of Crodamol STS significantly improved the performance of the conditioner system (figure 14).

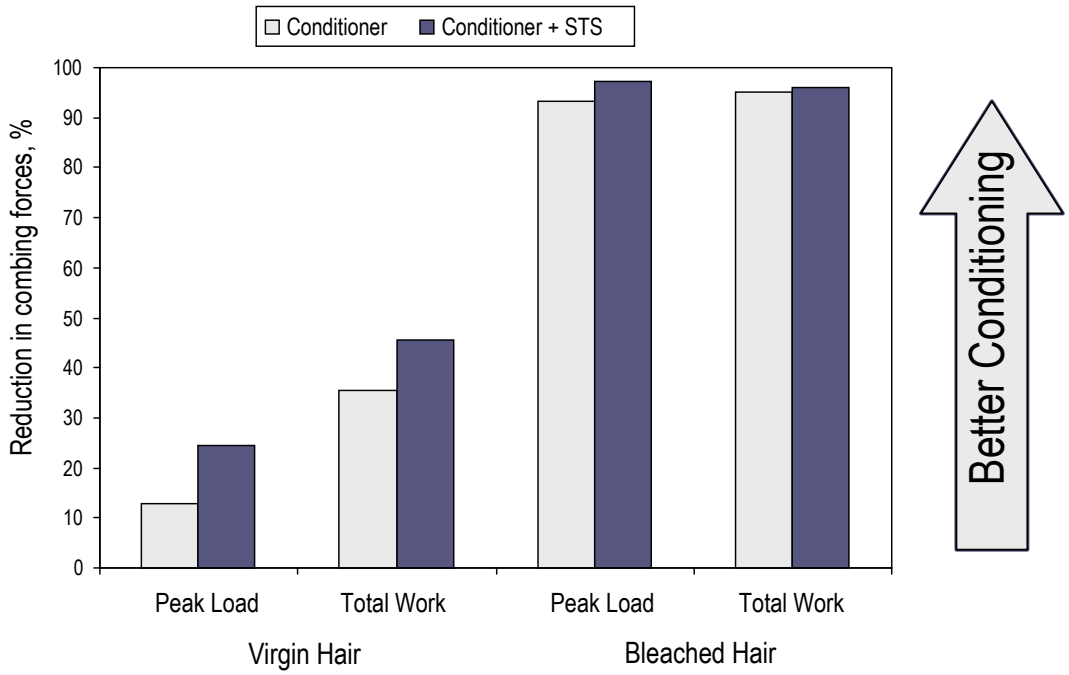


Figure: 14 Crodamol STS reduces combing forces

Hair Shine in Conditioning Systems

Previous studies from commercial shine products based on high silicone content such as shine sprays have demonstrated that Crodamol STS can be used to enhance the performance of these systems using moderate inclusion levels. This property was found to be transferable to conditioner systems, where the prototype conditioner containing Crodamol STS was found to deliver greater shine than the control system (figure 15).

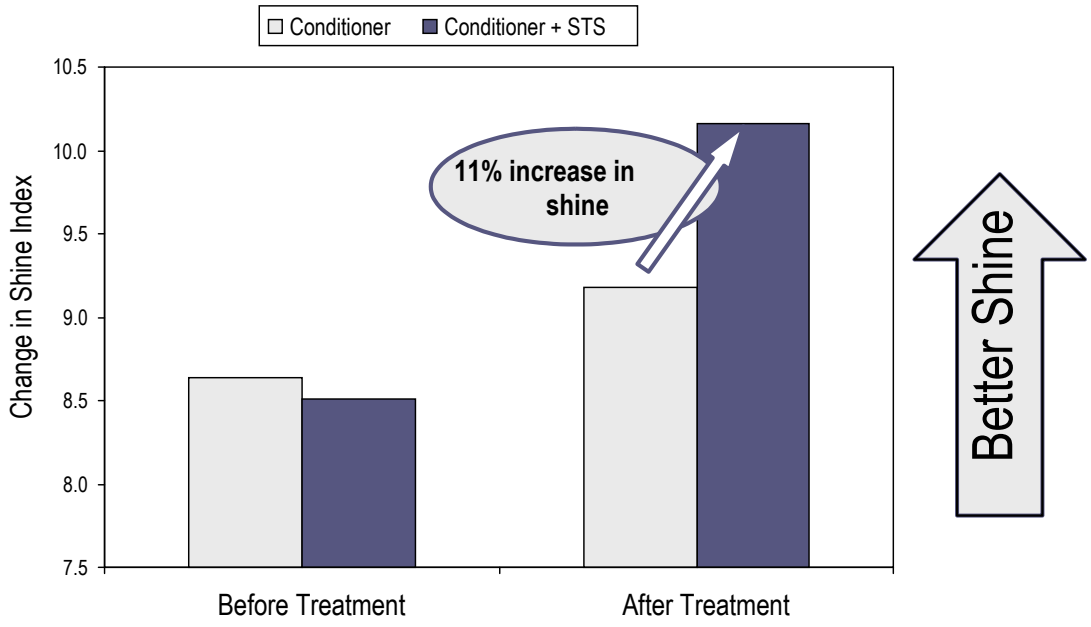


Figure: 15 Crodamol STS increases hair shine

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Assessment of Crodamol STS versus Silicone Fluids from Intensive Conditioning Treatments

Intensive conditioners are becoming increasingly popular for the treatment of damaged hair, particularly that which has undergone sever exposure to UV light or chemical treatments. The assessment of the performance of Crodamol STS as a functional alternative to silicones for use in conditioning treatments of this type has demonstrated that Crodamol STS is more effective for reducing both peak combing force and total work when compared to DC939 amidosilicone fluid.

Solubility

Solvent	Soluble	Dispersible	Insoluble
Alcohol SD 40	✓		
75/25 Alcohol/Water			✓
50/50 Alcohol/Water			✓
25/75 Alcohol/Water			✓
Deionised Water (pH 7.0)			✓
Deionised Water (pH 4.0)			✓
Deionised Water (pH 9.0)			✓
Crodamol PMP	✓		
Glycerin			✓
Propylene Glycol			✓
Ammonium lauryl Sulphate	✓		
SLES	✓		
TEALS	✓		
Mineral oil	✓		
Almond oil	✓		
DC 200 fluid		✓	
Cyclomethicone	✓		

Typical Analysis

Colour (APHA)	100
Acid Value	1.0-1.5
Saponification Value	102-109
Molecular Weight	495
Use levels	0.5-4%

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Regulatory

EINECS: Polymer
CAS: 403517-45-3

References

1. T. Maeda, M. Okada and T. Hara, Hair Luster, C&T Magazine, 107 (2), 1992.

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