

Crodafos™ BES-70

Crodafos BES-70 is a primary emulsifier based on phosphate ester chemistry. Crodafos BES-70 was especially designed with Behenyl chemistry to provide a unique sensory profile and like all Crodafos emulsifiers, provides excellent pH tolerance. It has exceptional body and contributes a rich, elegant feel to the initial rub-out of an emulsion.

Product	INCI name	Appearance
Crodafos BES-70	Beheneth-30 Phosphate (and) Cetostearyl Alcohol (and) Dicapryl Phosphate (and) Cetyl Phosphate	Pastille

Features / Benefits

- Extreme pH tolerance
- Versatility in formulating
- Behenyl chemistry
- Naturally substantive to skin
- High activity level

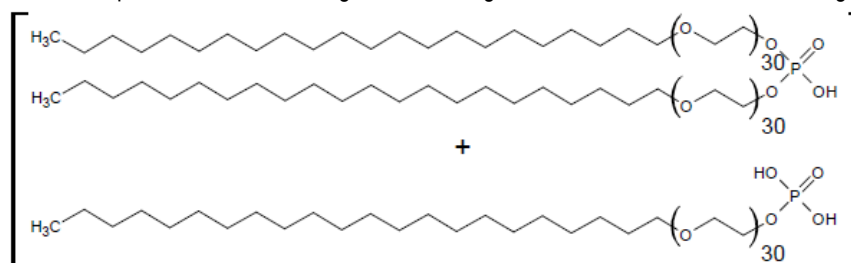
Applications

- Creams and lotions
- Anti-aging/treatment creams
- Sunscreens
- Self-tanners
- Anti-acne products

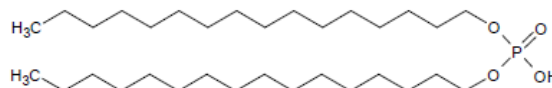
Phosphate Esters

As a phosphate ester, Crodafos BES-70 is similar in structure to the phospholipids found in the skin and is therefore substantive and compatible with the skin's natural lipids. Like phospholipids, di-alkyl phosphate esters have surfactant characteristics that tend to promote the formation of bilayers or lamellar structures. Such behaviour is thought to be the primary mechanism responsible for the enhanced oil deposition and delivery of actives onto the skin.

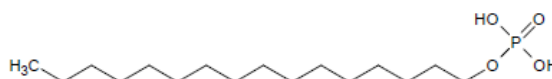
Formulations created with Crodafos BES-70 have extreme pH tolerance as the phosphate ester links, shielded by the alkyl chains, are stable at both high and low pH. Formulation stability can also be attributed to the large size of the lipid chains, shown in Figure 1, resulting in a combination of steric and charge stabilisation.



Beheneth 30 Phosphate



Di Cetyl Phosphate



Cetyl Phosphate
on™

Figure 1: Structure of Crodafos BES-70

Sensory Spectrum is a company that specialises in evaluating the specific sensory attributes of materials to assign quantitative measurement values to them. They have developed a set of Qualitative Descriptive Analysis Attributes (QDAA) that can be applied to raw materials and finished products. Using an expert panel, Sensory Spectrum apply a numerical value against each QDAA that can be directly correlated with consumer sensory perception data.

Statistical analysis of Sensory Spectrum data shows that 84% of an emulsion's appearance, pick-up and rub-out characteristics are dictated by the choice of emulsifier. Appearance describes the gloss and shape of the emulsion while pick-up and rub-out describe the initial skin feel. Understanding the strong correlation between the emulsifier and a product's initial sensory profile highlights the importance of choosing the right emulsifier at the beginning of the formulation development cycle. Pick-up and rub-out are the attributes that create the first impression of an emulsion for the consumer and are key in establishing product preference.

*Sensification is the understanding that **initial** skin feel, including pick-up and rub-out, is driven by the emulsifier.*

Crodafos BES-70 emulsions have a distinct sensory profile and to highlight this novel feel, Sensory Spectrum evaluated a number of simple emulsions including Crodafos BES-70, Crodafos CES and Crodafos CS20A. The formulations for these simple emulsions, referred to as 'Sensification™ Set Formulations', are detailed in the table below, followed by the Sensory Spectrum results.

Sensification Set Formulations

	Crodafos BES-70	Crodafos CES	Crodafos CS20A
Product/INCI Name	%w/w	%w/w	%w/w
Aqua	84.1	84.1	84.1
Crodafos™ BES 70 (Beheneth-30 Phosphate (and) Cetearyl Alcohol (and) Dicetyl Phosphate (and) Cetyl Phosphate)	1.8	-	-
Crodafos CES (Cetearyl Alcohol (and) Dicetyl Phosphate (and) Ceteth-10 Phosphate)	-	5.0	-
Crodafos CS20A (Cetearyl Alcohol (and) Ceteth-20 Phosphate (and) Dicetyl Phosphate)	-	-	5.0
Cetearyl Alcohol	3.2	-	-
Crodamol™ STS (PPG-3 Benzyl Ether Myristate)	10.0	10.0	10.0
Sodium Hydroxide (25% Aqueous Solution)	qs	qs	qs
Neolone 950	0.1	0.1	0.1
pH	5.5-6.5	5.5-6.5	5.5-6.5
Viscosity (cPs)	13,000	23,000	250

Table 1: Sensification Set Formulations evaluated by Sensory Spectrum.

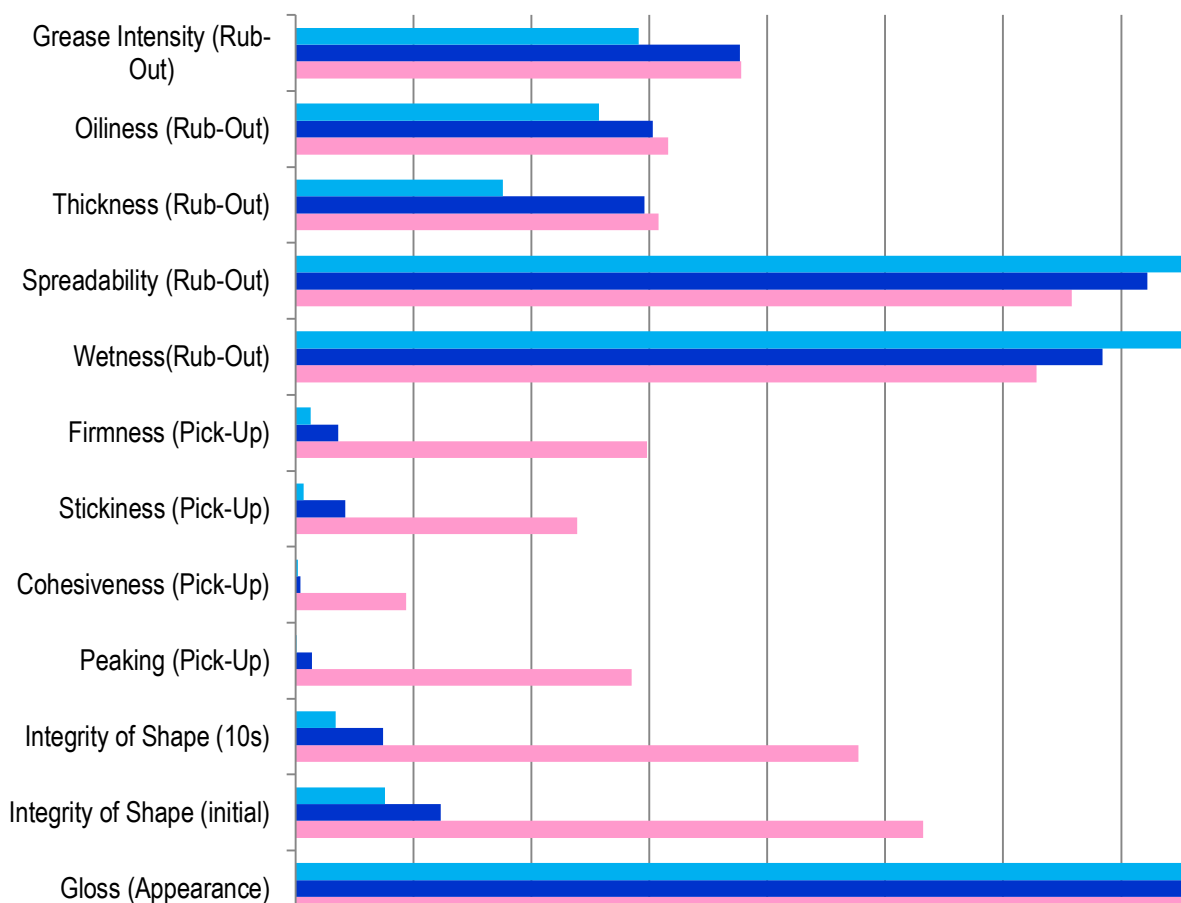


Figure 2: Sensory spectrum analysis of Crodafof BES-70, Crodafof CS20 A and Crodafof CES in an emulsion

There is a vast difference between the three Crodafof Sensification Set formulations, mainly in the categories of integrity of shape, peaking, stickiness, firmness, and spreadability. All of these results were statistically significant ($p < 0.0001$). The sensory profile of Crodafof BES-70 is unique and can be the first step in building a product with exceptional sensory characteristics.

Viscosity vs. pH Study

Crodafof BES-70 creates viscous creams at low pH with actives such as AHA and DHA. In order to test the relationship between the pH and viscosity of a typical emulsion we conducted the following study.

Test protocol

Simple emulsions were prepared with Crodafof BES-70 and neutralised to a pH between 4.5 and 12.5, while one formulation was left un-neutralised at a pH of 2.46. After 24 hours, the viscosity was measured using a Brookfield viscometer RV-TC @ 10rpm for 1 minute, and the pH reading was taken.

Crodafof BES-70 creates smooth, viscous emulsions across a large pH range, as seen in Figure 3, making it a perfect choice for formulations designed to deliver actives in an acid form such as salicylic acid or ascorbic acid. It is also well suited for high pH systems such as hair relaxers.

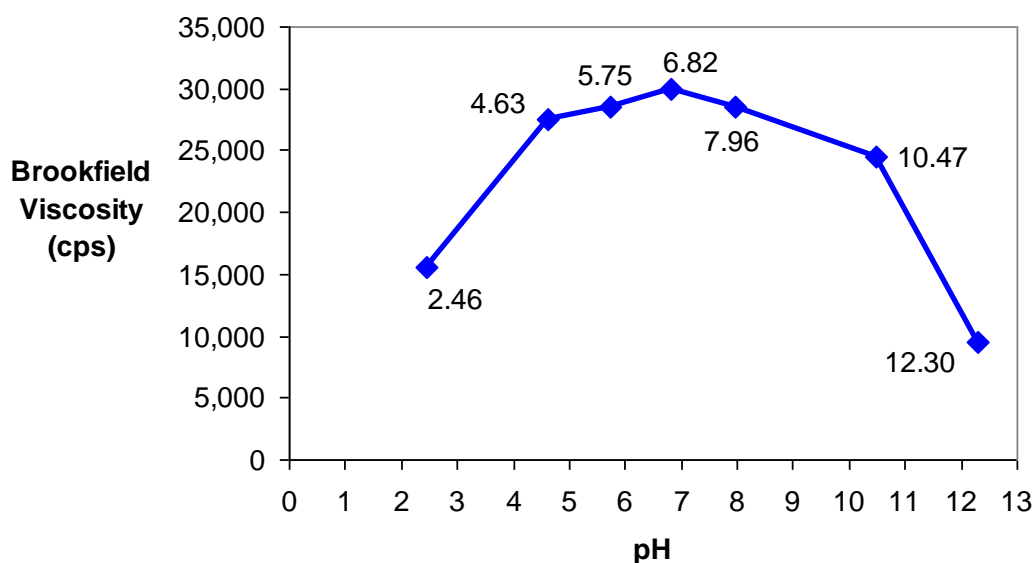


Figure 3: Crodafos BES-70 creates smooth, viscous emulsions across a large pH range as seen in the pH/viscosity curve

Self-Tanning

Two self-tanning formulations containing 4% DHA were created, one with Crodafos BES-70 and one with Glyceryl Stearate (and) PEG-100 Stearate as a benchmark. The objective was to analyse the difference in colour on the forearm of panellists following application of the two formulations using a Datacolor CHECKII.

Test Protocol

0.3 grams of each formulation (Table 2) was applied to a 2 inch circle on the panellists' volar forearms. Once dry, a baseline reading was taken using the Datacolor CHECK II spectrophotometer. Photos of the test areas were taken at 3 hours and 19 hours. Using a CIELabCH colour space model, the different components of colour were measured at at t=0, t=3 hours, and t=19 hours.

Ingredient	A	B
Product/INCI Name	%w/w	%w/w
PART A		
Water Deionised (Aqua)	73.75	74.00
Glycerin	4.00	4.00
Sodium Hydroxide, 25% Aqueous Solution	0.25	-
PART B		
Crodafos™ BES-70 (Beheneth-30 Phosphate (and) Cetostearyl Alcohol (and) Dicetyl Phosphate (and) Cetyl Phosphate)	1.80	-
Glyceryl Stearate (and) PEG 100 Stearate	-	4.00
Cetearyl Alcohol	3.20	1.00
Crodamol™ SFX (PPG-3 Benzyl Ether Ethylhexanoate)	3.00	3.00
Crodamol PMP (PPG 2 Myristyl Ether Propionate)	2.00	2.00
Theobroma Grandiflorum Seed Oil	2.00	2.00
PART C		
Arlasolve™ DMI (Dimethyl Isosorbide)	5.00	5.00
Dihydroxyacetone	4.00	4.00
PART D		
Germaben II	1.00	1.00
pH at 24 hrs	4.11	4.58
pH after 3 months	4.33	4.72

Table 2: Self-tanning formulations with Crodafos BES-70 or Glyceryl Stearate (and) PEG 100 Stearate

The results of the study in Table 3 show that the DHA formulation containing Crodafos BES-70 creates a darker and brighter, more intense colour on the skin in comparison to the control formulation.

	Panelist 1	Panelist 2	Panelist 3
Test Formulation A			
ΔL	-7.552	-6.842	-9.49
ΔC	7.966	9.212	10.888
Test Formulation B			
ΔL	-6.172	-5.548	-7.604
ΔC	8.024	8.182	9.122

Darker colour

Brighter colour

Table 3: Self-tanning results

L = light to dark

C = the deviation from grey (or chroma) – the higher the number, the lighter the colour

Formulating Guidelines

Crodafos BES-70 has the highest activity level of all the Crodafos phosphate esters. In order to build viscosity in the formulation, either carbomer, fatty alcohol or cellulose derivatives can be used. Building viscosity with one of these methods is essential for product stability. The ability to choose one or a combination of ingredients allows the formulator the highest degree of control over the formula's rheology.

Like Crodafos CES, Crodafos BES-70 requires neutralisation which can be done easily *in situ* with a variety of bases during the emulsion formation. The equation and table of neutralisation equivalents given below can be used to calculate the amount of base needed to neutralise Crodafos BES-70.

Grams of neutralising base per gram of Crodafos BES-70

$$(A.V. \bullet 0.70 \div 56100) \bullet X \bullet Y = \text{Grams. of base required}$$

A.V.= Acid value of Crodafos BES-70
(given in Certificate of Analysis)

X = Grams of product in formula

Y = Molar equivalent weight of base

If the acid value of Crodafos BES-70 is 85 and you are using 1.8% in the formula with NaOH (MW = 40) as the base, then the calculation would be as follows:

$$\frac{85 (0.70)}{56,100} \times (40) \times (1.8\%) = 0.076\% \text{ NaOH}$$

In the above example, you would need 0.067% NaOH in a 100% active basis to neutralise 2% Crodafos BES-70. The NaOH can be made into a solution for easy incorporation into the formula. The calculation can be done as a percent or as grams of product.

Neutralising Base	Molar Equivalent Wt. (Y)
TEA	149.19
KOH	56.1
NaOH	40.0
Ca(OH) ₂	37.05
LiOH	23.94

With a pH of around 3, Crodafos BES-70 is AHA-ready, meaning that it can produce stable emulsions within the low pH range in which AHAs must be formulated. This eliminates the need to add a neutralising agent to adjust the pH of Crodafos BES-70 during formulation.

Boost Your Day: SPF 30 Broad Spectrum Facial Sunscreen**C-5257****Ingredients****%w/w****Part A**

Deionised Water (Aqua)	58.58
Glycerin	4.00
Sodium Hydroxide, 25% Aqueous Solution	0.30
Disodium EDTA	0.10

Part B

Crodafos™ BES-70 (Beheneth-30 Phosphate (and) Cetostearyl Alcohol (and) Dicetyl Phosphate (and) Cetyl Phosphate)	1.80
Crodacol™ 1618 (Cetearyl Alcohol)	3.20
Syncrowax™ OSW (Tribehenin (and) Sorbitol/Sebacic Acid Copolymer Behenate)	2.00
Cromollient™ ESP (Tri(PPG-3 Benzyl Ether) Citrate)	3.00
Crodamol™ SFX (PPG-3 Benzyl Ether Ethylhexanoate)	2.00
Sensasil™ PCA (PCA Dimethicone)	1.00
Avobenzene	1.00
Oxybenzone	4.00
Homosalate	10.00
Octisalate	5.00
Octocrylene	0.80

Part C

SolPerform™ 100 (Water (and) Hydrolysed Wheat Protein/PVP Crosspolymer)	2.00
OptaSense™ RMA-IS (Sodium Polyacrylate (and) Caprylic/Capric Triglyceride (and) Mineral Oil (and) Tri(PPG-3 Myristyl Ether Citrate (and) Sorbitan Laurate (and) Trideceth-6)	0.22

Part D

Propylene Glycol and Diazolidinyl Urea (and) Propyl Paraben (and) Methyl Paraben ²	1.00
---	------

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

Viscosity- 13,840 cPs (Brookfield LVDVI+ Spindle 63 @ 6 rpm, at Room Temperature) Initial pH = 6.01

In-Vivo SPF: 32.70 (5 person panel, AMA Labs, New City, NY), Critical Wavelength = 372.3nm

192-2-086A, Control without Syncrowax OSW, In-Vivo SPF: 23.00 Critical Wavelength = 372.1nm

Procedure

Combine and mix Part A ingredients and heat to 70-75°C. Combine and mix Part B ingredients and heat to 70-75°C. With maintained heating and under low to moderate homogenisation, add Part B to Part A. Homogenize for several minutes and switch to propeller mixing with slow cooling. Mix Part C ingredients, once Part A/B reaches 35-40°C, add Part C. Add Part D and stir to room temperature. Check pH and adjust if necessary.

Clear Up Overnight Acne Cream**C-5258**

Treat your skin right with this comforting and soothing anti-acne treatment cream. Crodafos BES-70 creates a low spreading emulsion that is quickly absorbed into the skin.

Ingredients	%w/w
Part A	
Deionised Water (Aqua)	74.40
Crodafos™ BES-70 (Beheneth-30 Phosphate (and) Cetostearyl Alcohol (and) Dicetyl Phosphate (and) Cetyl Phosphate)	1.80
Disodium EDTA	0.10
Glycerin	4.00
Sodium Hydroxide, 25% Aqueous Solution	0.50
Part B	
Arlamol™ PS15E (PPG-15 Stearyl Ether)	8.00
Crodacol™ 1618 (Cetearyl Alcohol)	3.20
Part C	
Arlasolve™ DMI (Dimethyl Isosorbide)	5.00
Salicylic Acid	2.00
Part D	
Propylene Glycol and Diazolidinyl Urea (and) Propyl Paraben (and) Methyl Paraben ²	1.00
Suppliers: 1. Croda 2. Germaben II, Ashland	

Viscosity- 23,200 cPs (Brookfield HAT Spindle T-A @ 10rpm, at Room Temperature)

Initial pH = 3.20

Procedure

Combine and mix Part A ingredients and heat to 70-75°C. Combine and mix Part B ingredients and heat to 70-75°C. With maintained heating and under low to moderate homogenisation, add Part B to Part A. Homogenise for several minutes and switch to propeller mixing with slow cooling. Mix Part C ingredients, once Part A/B reaches 40-45°C, add Part C. Add Part D and stir to room temperature. Check pH and adjust to desired pH.

Sumptuous Self-Tanning Lotion**C-5259**

Treat yourself to a perfect tan with Crodafos BES-70. The behenyl chemistry of Crodafos BES-70 helps create a rich feeling lotion that is a pleasure to apply.

Ingredients	%w/w
Part A	
Deionised Water (Aqua)	73.75
Glycerin	4.00
Sodium Hydroxide, 25% Aqueous Solution	0.25
Part B	
Crodafos™ BES-70 (Beheneth-30 Phosphate (and) Cetostearyl Alcohol (and) Dicetyl Phosphate (and) Cetyl Phosphate)	1.80
Crodacol™ 1618 (Cetearyl Alcohol)	3.20
Crodamol™ SFX (PPG-3 Benzyl Ether Ethylhexanoate)	3.00
Crodamol PMP (PPG-2 Myristyl Ether Propionate)	2.00
Theobroma Grandiflorum Seed Butter	2.00
Part C	
Arlasolve™ DMI (Dimethyl Isosorbide)	5.00
Dihydroxyacetone	4.00
Part D	
Propylene Glycol and Diazolidinyl Urea (and) Propyl Paraben (and) Methyl Paraben ²	1.00

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

Viscosity- 9,660 cPs (Brookfield LVDVI+ Spindle 63 @ 6 rpm, at Room Temperature)

Initial pH = 4.72

Procedure

Combine and mix Part A ingredients and heat to 70-75°C. Combine and mix Part B ingredients and heat to 70-75°C. With maintained heating and under low to moderate homogenisation, add Part B to Part A. Homogenise for several minutes and switch to propeller mixing with slow cooling. Mix Part C ingredients, once Part A/B reaches 35-40°C, add Part C. Add Part D and stir to room temperature. Check pH and adjust if necessary.

Non-warranty

The information in this publication is believed to be accurate and is given in good faith, but no representation or warranty as to its completeness or accuracy is made. Suggestions for uses or applications are only opinions. Users are responsible for determining the suitability of these products for their own particular purpose. No representation or warranty, expressed or implied, is made with respect to information or products including, without limitation, warranties of merchantability, fitness for a particular purpose, non-infringement of any third party patent or other intellectual property rights including, without limit, copyright, trademark and designs. Any trademarks identified herein, unless otherwise noted, are trademarks of the Croda group of companies.

©2015 Croda International Plc