

Supplemental January 2009

Editor's note: The Surfactant Spectator[®] is always looking for articles that are of interest to our readers. No topic is more interesting to our readers than green surfactants, renewable resources, sustainable products and new technology.

We are very pleased to provide information on a new series of derivatives of alkyl polyglycosides (APG) that provide functionality to that green surfactant. This article is related to cationic versions of the APG molecule, but anionic, amphoteric and nonionic versions have been made and patented.

We believe that the quest for green products will lead to new technologies and new ways of thinking about products. The attached article is one such approach.

Happy reading. As always we are always interested to provide alternative thoughts and approaches.

Thomas O'Lenick Editor

New, Natural-based Quaternary Conditioners for Personal Care Applications

Robert J. Coots, Ph.D. Colonial Chemical, Inc.

ABSTRACT

Colonial Chemical has been conducting research aimed at developing new products for personal care applications that are natural, from sustainable raw materials, and that display improved toxicity relative to commonly used ingredients.

One of our first efforts in this area has led to a group of cationic products with broad application; these are called Suga[®]Quats. These cationic materials bring all of the quaternary-type benefits to a formulation: namely substantivity to skin and hair, and some anti-microbial benefits. But unlike the standard quaternary products (cetrimonium chloride - CTAC, Quaterniums) the products described in this article avoid all of the negatives. They don't interfere with the viscosity of the formulators' product, they don't affect the color in a negative way, they don't add irritation to formulations, and they don't suppress the foam.

Page 2

These new products, based on alkyl polyglucoside starting materials, show much less toxicity than standard quaternary products. The results indicate that these products are especially useful as conditioners in personal care products such as shampoos, conditioners, and body washes.

INTRODUCTION

Surfactant

We have been conducting research and development efforts toward the invention of new and improved cationic surfactants, useful as conditioners in a variety of personal care products.

There are numerous conditioners in the marketplace for personal care products, but most of these quaternium-type products have serious deficiencies. Most commercial products that claim to have conditioning effects in shampoo or conditioning formulations, have one or more deleterious effects on the overall formulation. These negative effects include reduction of viscosity and decrease in foaming, among others. In addition, the potential for irritation to human skin or eyes can be very substantial for many of these products.

The products that are the subject of this paper overcome many of these effects. These quaternium products are based on alkyl polyglucoside (APG) precursors, and retain much of the properties of these versatile nonionic surfactants. When the APG molecules are derivatized with lauryl or stearyl dimethylquat groups, the resultant cationic products have good foaming, solubility, and viscosity properties.

The APG precursors bring many positive attributes to these products. They are based on renewable raw materials. They are extremely mild. They are readily biodegradable and are safe for the environment. They are viscosity enhancers. They have good cleansing power. They modify rheology in positive ways. They have substantivity to the hair. They are stable over a wide pH range.

However, once the APG has been derivatized into a cationic surfactant, many of these attributes are dramatically enhanced. The foam properties are improved, they have even less irritation, and their solubility is greatly enhanced.

The viscosity response in a standard shampoo formulation is much more favorable than when using traditional quat conditioners. The toxicity profiles of the Suga[®]Quat products are much improved compared to CTAC or benzalkonium chloride (BAC). In addition, these products are biodegradable, and are produced from renewable, natural plant sources.

Surfactant Spectator

Silicone Spectator P.O. Box 715 Dacula, Ga 30019 Andrew O'Lenick Editor Page 3

METHODS

Synthesis



The variation in structure of these molecules gives the formulator a variety of products from which to choose. The alkyl portion of the APG molecule can vary, not only from the C8-C16 range of coconut derived fatty alcohols, but can also be a butyl group, or 2-ethylhexyl group. There is also the possibility for variation in the quat group: lauryl dimethyl, stearyl dimethyl, or trimethyl.

The typical physical properties of selected Suga[®]Quat products are shown in Table 1 below. These products are supplied at about 30% solids in a water solution. The color of the products is about 1 Gardner, which makes these well suited for clear shampoo or body wash products. The Suga[®]Quat products are supplied at pH range of 6 - 8.

The data in this table includes Draves wetting, and it can be seen that these products have good wetting properties when diluted to 1% active solutions. In addition, these products are generally soluble in 25% NaOH and 25% H_2SO_4 . There is no indication of instability of these products at these extreme pH levels.

The Suga[®]Quat products are also generally compatible with anionic surfactants such as SLS and DSLS (disodium laureth sulfosuccinate). This is an important feature because these cationic products are typically blended with anionic surfactants to prepare conditioning shampoos or body wash products.

Silicone Spectator Andrew O'Lenick P.O. Box 715 Dacula, Ga 30019

	L-1010	L-1210	S-1010	S-1210
Color, Gardner	< 1	1	< 1	1 +
Activity, %	30.8	29.7	29.1	30.5
Viscosity, cps (as is)	16	106	21.5	9800
Odor	mild fatty odor	mild fatty odor	mild fatty odor	mild fatty odor
pH(10% aq.)	6.70	6.99	6.76	7.12
Appearance, 10% solution	clear	clear	clear	clear
Draves Wetting (1 % active)	4	9	15	15
Solubility, 10% active solution 25% NaOH 25% H ₂ SO ₄	clear (gel) Soluble	clear (gel) soluble	soluble soluble	clear (gel) soluble
Compatibility, 5% active solution				
	Clear at 1:1	Cloudy at 1:1	Soluble, all	Clear at 1:1
5% active SLS			ratios	
	Soluble, all	Cloudy at 1:5	Clear at 1:1	Cloudy, all
5% active DSLS	ratios	(thickens)	(thickens)	ratios

Table 1. Typical Properties

FOAMING PROPERTIES

The foaming properties of several of the Suga[®]Quat products were tested by an independent laboratory.¹ The results are shown graphically in Figures 1 and 2. The first graph shows initial foam height for several surfactants, including sodium lauryl sulfate (SLS) and sodium laureth sulfate (SLES) against the Suga[®]Quat products and one of the APG precursors. It is readily apparent that Suga[®]Quat L-1010 gives nearly as much foam as SLS, and more foam than SLES. The other Suga[®]Quat products all give improved foam over the APG precursor.

In Figure 2, the foam structure is evaluated using a foam density test. Suga[®]Quat L-1010 and L-1210 both perform quite well in this test; in fact the L-1010 product actually outperforms SLS.

Surfactant Spec

Silicone Spectator P.O. Box 715 Dacula, Ga 30019

Andrew O'Lenick Editor Page 5



Figure 1. Initial Foam Height



Figure 2. Foam Density Test

Surfactant Spectator

Silicone Spectator P.O. Box 715 Dacula, Ga 30019 Andrew O'Lenick Editor Page 6

VISCOSITY EFFECTS

Figure 3 shows a graph of a salt – viscosity curve for a typical shampoo formulation, using two Suga[®]Quat products and CTAC. Clearly, there is significantly more viscosity reduction when using the cetrimonium chloride product versus Suga[®]Quat. This effect is seen even more clearly at a 6% level of quat, as shown in Figure 4.



Figure 3. Salt - Viscosity curve, 2% Quat

Surfactant Spectator

Silicone Spectator P.O. Box 715 Dacula, Ga 30019

Andrew O'Lenick



Figure 4. Salt – Viscosity curve, 6% Quat

TOXICITY_PROFILES

The Suga[®]Quat products have been tested by an independent, outside laboratory, and are shown to be safe materials when used in combination with other personal care raw materials. These products have been evaluated for eye and skin irritation. The results are summarized below.[#]

Eye Irritation

Suga[®]Quats were tested for eye irritation using the chorioallantoic membrane technique (HET-CAM). The test was performed with the cationic surfactant diluted to 2% activity. This test utilizes the inner membrane of a hen's egg to gauge the irritation potential of a compound by visual observation of injurious changes in the membrane.

Page 7

Andrew O'Lenick Editor



Figure 5. HET-CAM test results

The results of the HET-CAM eye irritation are shown in Figure 5. Clearly, Suga[®]Quat S-1210 has much less eye irritation than Suga[®]Quat L-1210 and Suga[®]Quat L-1010. All of the Suga[®]Quat products, however, show significantly less irritation as compared to cetrimonium chloride, or stearalkonium chloride. The Suga[®]Quat products also have less irritation than the primary surfactant, SLS, and in the case of S-1210, less than a popular brand of baby shampoo.

Skin Irritation

To evaluate the potential irritation to skin, a patch test study was performed adhering to ICH Guideline E6 and 21 CFR parts 50 and 56. A 1" by 1" absorbent pad was moistened with 0.2 ml of liquid and applied to the backs of the subjects between the scapulae. The patch sites were inspected at 48 hours for gross changes. It was observed that there was a complete absence of skin change. The test sites were evaluated again at 72 hours. Once again the observation was negative skin changes. Under the conditions of this test, Suga[®]Quat products did not indicate a potential for dermal irritation.

It is documented in published literature that stearalkonium chloride and cetrimonium chloride both show a high potential for dermal irritation.^{III}

Biodegradability

Surfactant

Biodegradability of the Suga[®]Quat products are expected to be good, as the APG precursors show very good biodegradability. The quaternary ammonium portion of the molecule is also known to have good biodegradability.[™]

In addition, the APG precursors are known to have low environmental toxicity.^v

APPLICATIONS

The Suga[®]Quat products show excellent compatibility with other ingredients in personal care formulations, and are substantive to the skin and hair. They also have low levels of irritation, and can be used in formulations that call for conditioning of skin or hair.

- Skin Care Products: creams, lotions, tonics, shower gels, etc.
- Hair Care Products: shampoos, conditioners, hair tonics, hair creams, etc.
- Sun Care Products: pre and post sun care creams, lotions, gels, etc.
- Make-up Products: foundations, lipsticks, etc.
- Health Care

CONCLUSIONS

We have created cationic surfactants that bring all of the quat type benefits to a formulation, namely substantivity to skin and hair, along with some antimicrobial benefits. But unlike the standard quats (CTAC, parabens, Quaterniums) our products avoid all of the negatives. They don't interfere with the viscosity of the formulators' product, they don't affect the color in a negative way, and they don't add irritation to formulations. They don't suppress the foam, on the contrary, most of them boost the foam.

The combined attributes of these cationic surfactants give the formulator of personal care products a valuable tool to use when putting together products that require conditioning with low irritation, good biodegradability, and renewable resources. In other words, these are an obvious choice for Green formulations.

ⁱCosmetech Laboratories, 39 Plymouth St., Fairfield, NJ 07004, USA.

- ⁱⁱ Consumer Product Testing Company, 70 New Dutch Lane, Fairfield, NJ, 07004, USA.
- ⁱⁱⁱ BASF, M-QUAT® DIMER 18 QUATERNARY AMMONIUM COMPOUND, Technical Bulletin.

^{iv} Surfactant Biodegradation, Robert Donald Swisher, Published 1987, Marcel Dekker, p. 500.

^v Seppic, APG Biodegradability technical bulletin.

Surfactant Spectator[®] is a registered trademark of SurfaTech Corporation. All rights reserved.