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Anionic / Cationic Complexes

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There have been a multitude of approaches to the formulation of hair care products that provide multi-functional benefits. This is due in part to the fact that the various functions we expect from our multi-functional products do not co-exist well in one formulation. Specifically, the consumer demands cleansing, viscosity, foam, wet conditioning (antistat and wet comb), and longer term conditioning (dry property conditioning). It would be ideal if there a universal surfactant existed that had just the right amount of each property so formulation would be easy. Alas, there is no universal surfactant. Any step toward increasing the level understanding related to the interaction of surfactants and providing optimized properties in formulation is desirable.

One major area in which interactions are critical is the Anionic / cationic interaction. Most formulators of two in one shampoos understand that indiscriminate mixing of anionic and cationic materials can result in undesired insoluble gunky solids. We have classified anionic and cationic materials that are incompatible when mixed together as *hard complexes.* As the expression implies the cationic and anionic compound possess properties which when added together form insoluble complexes (salts). In contrast, anionic and cationic compounds that can be mixed over a wide range of ratios and provide a clear viscous high foaming complex are defines *as soft complexes.* Optimized soft complexes have many desirable properties including high levels of foam, viscosity build without alkanolamides, conditioning properties and low levels of eye and skin irritation.

The terms used for quats and anionic materials are an adaptation of the work of Pearson used to describe acids and bases. Pearson proposed that “hard acids bind strongly to hard bases and soft acids bind softly to soft bases”[2], the anionic and cationic interactions are exactly analogous. (Pearson R.G. Pearson, *J Am Chem Soc*, **85**, 335 (1963)

The structural changes that can be made to cationic molecules can “soften” them, making them more compatible with anionic systems. The compatibility of specific quats with sodium lauryl sulfate (SLS) and sodium laureth-3-sulfate (SLES), the foam properties of the combinations with SLS and SLES and the substantivity of these combinations with SLS and SLES are key factors in understanding the function of conditioners.

In order to understand the interaction the following quats were studied in combination with SLS and SLES-3:

$$
\begin{array}{c}
R^2 \\
| \\
R^1\text{-}N^+\text{-}R^3 \qquad Cl^- \\
| \\
R^2
\end{array}
$$

R^1
1. Alkyl (C12)
2. Ricinoleylamidopropyl
3. Dilinoleylamidopropyl
4. Cocamidopropyl
5.

R^2
1. Methyl $-CH_3$
2. 2-hydroxy ethyl $-CH_2CH_2OH$

R^3
1. Methyl $-CH_3$
2. Benzyl $-CH_2-C_6H_5$
3. Glyceryl $-CH_2-CH(OH)-CH_2-OH$

Table 1 Compounds Studied

Name	R^1	R^2	R^3	Description
AMB	Alkyl (C12)	CH_3	Benzyl	Coco dimethyl benzyl ammonium chloride
AME	Alkyl (C12)	CH_2CH_2OH	CH_3	Coco di-2 hydroxyethyl methyl ammonium chloride
AMG	Alkyl (C12)	CH_3	Glyceryl	Coco dimethyl Glyceryl ammonium chloride
AMM	Alkyl (C12)	CH_3	CH_3	Coco tri-methyl ammonium chloride
AEB	Alkyl (C12)	CH_2CH_2OH	Benzyl	Coco di-2 hydroxyethyl benzyl ammonium chloride
AEG	Alkyl (C12)	CH_2CH_2OH	Glyceryl	Coco di-2 hydroxyethyl glyceryl ammonium chloride
CaMB	Castor Amido	CH_3	Benzyl	Ricinoleylamidopropyl dimethyl benzyl ammonium chloride
CaMG	Castor Amido	CH_3	Glyceryl	Ricinoleylamidopropyl dimethyl glyceryl ammonium chloride
DMB	Dimer Amido	CH_3	Benzyl	Dilinoleylamidopropyl dimethyl benzyl ammonium chloride
DMG	Dimer Amido	CH_3	Glyceryl	Dilinoleylamidopropyl dimethyl glyceryl ammonium chloride
DMM	Dimer Amido	CH_3	CH_3	Dilinoleylamidopropyl trimethyl ammonium chloride
MMB	Cocamido	CH_3	Benzyl	Cocamidopropyl dimethyl benzyl ammonium chloride
MMG	Cocamido	CH_3	Glyceryl	Cocamidopropyl dimethyl glyceryl ammonium chloride
MMM	Cocamido	CH_3	CH_3	Cocamidopropyl trimethyl ammonium chloride

Test Methodology

(A) Compatibility with anionic

A determination of compatibility of a variety of quats with two anionic surfactants, sodium lauryl sulfate and sodium laureth-3-sulfate was made. The compatibility was determined by titration. The point at which an anionic solution containing 10% anionic either became hazy formed a precipitate was determined.

1. Prepare a 10% active solution of SLS and SLES.
2. Prepare 100g of a 10% active test solution for each quat sample.
3. Add 100g of a 10% solution of sulfate to a 250 ml beaker.
4. Under good agitation, titrate the solution with the 10% quat.
5. The endpoint is (a) first sign of an insoluble complex, (b) haziness or (c) viscosity build.

RESULTS

The quats which were compatible with SLS or SLES-3 are shown in table 2. All others in the study group were incompatible.

Table 2
Soft Quats – Gel Formers
(100 g of 10% solution of anionic, titrated with 10% solution of quat)

Quat Sample	**Soft quats in SLS (viscosity of gel)**		**Quat Sample**	**Soft quats in SLS-3 (viscosity of gel)**
MMB	14,000		AME	7,000
MMM	13,400		DMM	6,200
DMM	6,000		MMM	50,000
CaMB	1,000		CaMB	1,000
MMG	19,200		AMG	1,000
DMG	12,000		MMB	9,800
			MMG	40,000
			DMG	6,800
			AEG	1,000
			CaMG	1,000

Foam Testing

The solutions shown above were cut with water to 1% active and evaluated in cylinder shake foam tests. The foam data is shown in table 2.

Table 2
Foam Heights
(Cylinder Shake Foam Test)

Quat Sample	**Foam Height (mL) (SLS)**	**Foam Height (mL) (SLES)**
AMB	Does not foam	Does not foam
AME	190	90
AMG	500	400
AMM	600	500
AEB	300	200
AEG	200	100
CaMB	250	150
CaMG	200	100
DMB	400	300
DMG	300	200
DMM	250	150
MMB	400	300
MMG	400	300
MMM	400	300
Control No Quat	600	450

CONCLUSIONS

Quaternium compounds can be classified as hard or soft by their ability to form gelled systems with anionic systems. Cationic systems that form a gel at near stoichiometric amounts are classified as “soft”, those that form precipitates of haze without appreciable viscosity build up are classified as “hard” quats. “Soft quats” can produce foam in the systems they gel, albeit at levels below the volume of foam generated by the anionic, per se.

Quaternium compounds titrated with sodium laureth-3-sulfate (SLES) produced greater viscosities with amido quats. The exception was amido quats containing a benzyl group, which exhibited a low viscosity in SLES.

Good foaming results were also seen with a number of complexes. Additional work needs to be done to expand the testing to a variety of compounds including silicone based compounds.

This study was sponsored by Phoenix Chemical (Somerville N.J.) and SurfaTech Corporation (Dacula, Ga). It was conducted by Thomas O’Lenick a graduate student pursuing a PhD at The University of Tennessee (synthesis) and Tim Brockman is a senior Chemistry major at Bloomsburg College (evaluation).