



Qualitative and quantitative interactions of cationic surfactants with cosmetic anionic ingredients

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Introduction of research

Surfactants are known for their detergency properties and are part of many cosmetic applications. On top of this characteristic displayed by anionic surfactants, cationic surfactants on the other hand are also used as broad-spectrum antimicrobial agents.

There is a well spread belief that anionic species would systematically interact with cationic surfactants, thus inhibiting their efficiency and leading to some sort of automatic incompatibility. The present study aims at revisiting this belief using scientific tools targeting the establishment of objective conclusions.

Isothermal Titration Calorimetry (ITC) is a well-known technique in the biomolecular field, that quantitatively determine the thermodynamic parameter of molecular interactions [1-2]. Conductimetric methods have been used to characterize ionic surfactants behavior in solution [3].

The research purpose was to develop a methodology using physico-chemical tools to determine the degree of interactions between cationic preservative species and anionic compounds and to achieve a proper selection of cationic preservative to a given cosmetic formulation, in presence of anionic surfactants.

Results and discussion

The molecular interactions were investigated by monitoring the conductivity of 1:1 molar ratio of Didecyldimethylammonium chloride (DDAC) and anionic surfactants. Figure 1 shows the 'measured to theoretical' conductivity ratio for each pair. Increasing the concentration of the molecules increased the 'measured to theoretical' conductivity ratio. At 10mM of each molecule the majority of the 'measured to theoretical' ratio values exceeded 100%. The conductance behavior of the combined molecules (*i.e.*, measured) is expected to differ from the sum of the individual component solution's (*i.e.*, theoretical) once molecular interactions molecules take place. The stronger the molecular interactions are, the larger the deviation is expected to be.

Mixtures of DDAC and anionic molecules having sulfate or sulfonate functional group exhibited conductivity profiles with higher slopes compared to DDAC and carboxylate pairs.

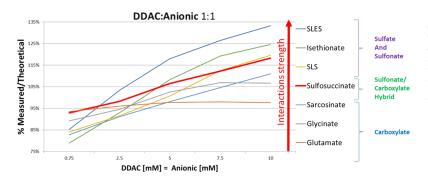


Figure 1: 'Measured to theoretical' conductivity ratio for each DDAC:anionic surfactant pair (1:1 molar ratio) at the concentration range of 0.75-10mM (at 25°C).



The molecular interactions between the cationic DDAC and various anionic molecules were further detected by ITC. The binding process could be directly measured by monitoring the heat evolution due to the molecular interactions, thereby determining the values of the binding constant (Ka), the stoichiometry (n) and the enthalpy of binding (Δ H) [2]. The integrated data of the enthalpy variation (Δ H) per mole of DDAC are plotted vs. the DDAC/anionic surfactant molar ratio (Figure 2). The measurements indicate a distinct difference in the behavior of anionic surfactants having a sulfate or sulfonate group when mixed with DDAC (higher enthalpy changes) in comparison with anionic surfactants bearing a carboxylate group.

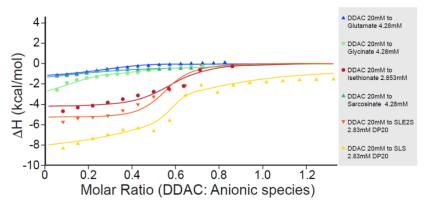


Figure 2: Enthalpy change per injection *vs.* DDAC/anionic surfactant molar ratio. DDAC was injected into a reaction cell containing different aqueous anionic solutions at RT.

In order to corroborate the above results with the antimicrobial efficacy of cationic surfactants, the challenge tests shown in Table 1 were performed, with the cationic preservative surfactant (0.5% of the total final product) within the designated cosmetic anionic shampoo.

Two pairs of anionic and cationic surfactants were selected, SLES/DDAC and Glutamate/Polyquaternium-80, representing the strongest and weakest interactions. Strong ionic interactions of sulfate-based molecules and DDAC led to a failed challenge test, while weak interactions between carboxylate-based molecules and P-80 did not interfere with the cationic antimicrobial activity which resulted in passing the challenge test.

Composition	Time	E.Coli (Gram- Bacteria)	C. albicans (Yeast)	Composit
Anionic surfactant in Shampoo: SLES Cationic surfactant in preservative: DDAC	Inoculum	1.1x10^6	1x10^5	Anionic surf
	2 days	2x10^5	1x10^5	in Shamp
	7 days	2x10^5	1.8x10^3	Glutama
	14 days	2x10^5	2.5x10^2	Cationic surf
	21 days	2x10^5	<10	in preserva
	28 days	2.6x10^5	<10	P-80

Composition	Time	E.Coli (Gram- Bacteria)	C. albicans (Yeast)
Anionic surfactant	Inoculum	1.1x10^6	1x10^5
in Shampoo:	2 days	<10	<10
Glutamate	7 days	<10	<10
Cationic surfactant	14 days	<10	<10
in preservative:	21 days	<10	<10
P-80	28 days	<10	<10

Table 1: Challenge tests of 0.5% preservative mixtures containing DDAC or Polyquaternium-80 in anionic shampoo cosmetic formulation containing SLES or Glutamate, respectively.

Conclusion

This study reveals that far to be a systematic phenomenon, not all anionic species would interact with cationic surfactants but only a specific subgroup. The tools developed allow to quickly assess and predict the interactions between any anionic and cationic species with reliability.

This innovative work opens a new window of opportunities for ingredients selection based on the scientific understanding of the molecular interactions.

References

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About the speaker

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Dr. Paul Salama holds a B.Sc. in Chemistry and a M.Sc. in Chemical Engineering both from University of Lyon (France), along with a Ph.D. in Organic Chemistry from University of Montreal (Canada).

After having started his career as a university professor in Canada, he moved to the pharmaceutical industry in Canada then in Israel, holding senior research positions (VP CMC).

Dr. Salama leads the R&D activities of Sharon Laboratories since 2014 as its CTO and Head of Innovation.