Fragrance: The Most Chemically Complex Additive to Cosmetic Formulations

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INTRODUCTION

Fragrance, as an ingredient, is oftentimes perceived as a single component in a cosmetic product, when in fact it is usually the most chemically complex additive to the formulation. The composition of a fragrance can reach well over one hundred compounds, which include essential oils and their isolates as well as other synthetically derived aroma chemicals. Although fragrances are designed for a wide variety of applications, they are not indefinitely stable. Interactions between fragrance and base can undergo a number of reactions, many of which can result in undesirable changes to a product's solubility, clarity, color, viscosity, or pH. Environmental conditions like temperature, humidity and light often accelerate these reactions and are simulated in a lab to predict the compatibility and stability of fragrances in application. This paper reviews the basic foundation of fragrance chemistry and discusses common interactions of aroma chemicals in cosmetic formulations.

FUNCTIONAL GROUPS

Fragrance molecules have a backbone of carbon and can bond to one another to form an almost infinite array of molecular structures. Functional groups that are most relevant to fragrance chemistry consist of carbon, hydrogen, oxygen, nitrogen, and sulfur and are the part of the molecule that interacts with its surroundings. Consequently, they are also the part of the molecule most susceptible to chemical change. The carbonyl group (C=O) can undergo several reactions that interfere with other base ingredients including oxidation, reactions with other acids, and addition reactions. Fig. 1 gives a few examples of fragrance ingredients and their corresponding functional groups.

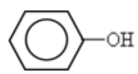
ALCOHOLS	—OH	Menthol Terpineol Phenyl Ethyl Alcohol	**ESTERS**	—C(=O)—O—	Iso amyl acetate Cis-3 Hexenyl Acetate Benzyl Salicylate
PHENOLS		Vanillin Eugenol Thymol	**ETHERS**	—O—	Diphenyl Ether Rum Ether Para Cresyl-Methyl Ether
ALDEHYDES	—C(=O)—H	Benzaldehyde Anisic Aldehyde Cinnamic Aldehyde	**NITROGEN COMPOUNDS**	—N(—)—	Methyl Antranilate Indole Aurantiol
KETONES	—C(=O)—	Floralozone Menthone Iso Jasmone	**SULFUR COMPOUNDS**	—S—	Dimethyl Sulfide Thiomenthone Furfuryl Mercaptan

Figure 1 Illustrates Several Functional Groups Relevant to Fragrance Chemistry

SOLUBILITY

The saying *like dissolves like* holds true for fragrance compounds. Since aroma molecules range in polarity, solvents are used to influence the overall polarity of the fragrance. Where a polar solvent is needed for hydrophilic bases like shampoo or body wash, a non-polar solvent would be appropriate for lipophilic bases like lipstick or styling wax. If the fragrance is not soluble in a specific base, usually the solvent system of that fragrance can be readily interchanged to be compatible in such polar and non-polar conditions. However, in systems that are comprised almost entirely of water, a polar solvent may not be enough to achieve a soluble product. Non-ionic surfactants are incorporated into fragrances that require complete water solubility. A simple freeze/thaw test can be used to best predict whether a fragrance will remain soluble in product over time.

CLARITY

Fragrance ingredients consisting of hydrocarbons with long non-polar chains have limited solubility in aqueous and alcoholic systems. Even with a solubilizer, they do not dissolve as readily in such polar conditions and cause haziness, opaqueness or possibly separation from product. Cosmetic formulations that are comprised almost entirely of silicones or mineral oil are extremely lipophilic and with the addition of a fragrance will oftentimes lose clarity. Even with a non-polar solvent, any polar aroma chemicals within the fragrance will cause a slight haze to appear. Haziness can be minimized by having the least amount of polar aroma chemicals in the fragrance or reducing the amount of silicones or other petroleum-based ingredients in the finished product. Alternatively, for non-transparent products, incorporating an emulsifier into the final formulation, in which case clarity becomes extraneous, is usually the most logical solution.

COLOR

The oil of the fragrance is usually difficult to de-color without changing the scent or integrity of that fragrance. If used at small concentrations, a fragrance may not appear to have any effect on the overall color of the finished product; however there are several aroma chemicals that may discolor over time. Citrus and vanilla aroma chemicals are the most susceptible to darkening of a product due to how readily they oxidize. Their effects depend on the other base ingredients and product packaging, and can be diminished using antioxidants, preservatives and avoiding exposure to light (e.g. dark, non-transparent container). Other aroma chemicals react directly with the dye molecules and can cause a bleaching effect to occur. Oftentimes, a UV absorber is formulated into the fragrance to prevent the product from discoloring. Heat and UV light are used to test a product's stability by accelerating any reaction the fragrance may undergo that would cause color change in the finished product.

VISCOSITY

The salt curve is commonly used to adjust viscosity in surfactant-based applications. The salt, an electrolyte, will increase the size of the micelles and compete with surfactants for water, increasing viscosity. The addition of a fragrance blend can shift the salt curve and disrupt the product's desired viscosity. The polarity within a fragrance may compete for space in emulsion systems, consequently lead to the breaking of an emulsion and cause complete viscosity loss of the fragranced product. The solvent or solubilizer can influence the viscosity of the final product, but many times the removal of some problem fragrance ingredients or the addition of a viscosity modifier is necessary.

PH

The pH of the fragrance oil and the pH of the finished base are important when discussing product stability. The addition of a fragrance may alter the pH of the final formulation or even worse, disrupt the product's functionality. Additionally, several reactions are observed when aroma chemicals are introduced to acidic or basic conditions. The more deviation from a neutral pH, the more likely the degradation of fragrance ingredients will be. Needless to say, the more extreme the pH of the product formulation, the less stable fragrance ingredients can be used, limiting the sophistication of many pH stable fragrance types.

DISCUSSION

Fragrance interactions vary in different environments which can lead to unforeseen product issues over time. There are many other factors to consider like base odor, packaging of the product, storage conditions, or other actives that will have an impact on the fragrance's stability and longevity. Collaboration amongst formulators, marketers, and perfumers are essential during product development so that a fragrance can be formulated for maximum stability in its intended application. Fragrance is chemistry and understanding some of these technical aspects is crucial for developing a stable finished product and achieving commercial success for fragranced cosmetics in the personal care industry.