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Trans Isomers in Cosmetics

[Soap & Cosmetics](#)

Cosmetic chemists may soon be called upon to identify the trans isomer content of their brand's formulations and to certify that their products are "Trans Free." The impetus behind the movement is in part due to consumer concerns that trans fatty acids are not healthful in their diets and will be undesirable to use on their body as well. This intuitive reaction is not without merit. Trans fatty acids have been implicated in the inhibition of Δ^5 and Δ^6 desaturation of polyunsaturated fatty acids; i.e., the metabolic pathway to prostaglandin formation. Prostaglandins are important mediators of skin metabolism. Topical introduction of trans fatty acids may disrupt normal prostaglandin formation.

The fire is also being stoked in the USA due to broad new FDA food labeling proposals (World Food Chemical News, November 24, 1999, Volume 6, Number 16) that would require the amount of trans fatty acids in a product to be listed on the "Nutrition Facts" panel of food labels. This trans fatty acid isomer phenomenon is the latest "food borne" trend to be transposed to cosmetics. Marketers will undoubtedly find a receptive audience for claims of "Trans Free" cosmetic and personal care products. The good news is that trans isomers are easy to detect, there are alternative routes to obtain "Trans Free" ingredients and naturally occurring trans isomers are rare.

CIS AND TRANS GEOMETRY

The cis and trans labels refer to the geometric positioning of hydrogen atoms about points of unsaturation (double bonds) found in lipid chains. The cis isomer is simplistically represented by both hydrogen atoms of the carbon atoms forming the double bond being located on the same side of the carbon chain (See Figure 1). The trans form is depicted with hydrogen atoms appearing on opposite sides of the carbon chain (See Figure 2).

NATURE MAKES CIS FATTY ACIDS

Nature creates an overwhelming majority of cis fatty acids (and fatty alcohols) as components of lipid materials (emollients) such as vegetable oils, fats, wax esters, etc. Trans isomers of lipid materials occur infrequently in nature. Table 1 contains a listing of some of the relatively rare sources of naturally occurring trans fatty acid isomers. Non-natural trans isomers are usually formed when lipid materials are subjected to various chemical transformations such as partial hydrogenation, oxidation, transisomerization, or certain enzymatic reactions.

TRANS ISOMERS INHIBIT PROSTAGLANDIN SYNTHESIS

In vivo studies [1,2] using human skin cells have shown that some monoene trans fatty acids inhibit both Δ^5 and Δ^6 desaturation of fatty acids. This synthesis pathway in humans to important prostaglandins require that the essential fatty acids, linoleic and linolenic acids, be first Δ^6 desaturated to γ -linolenic and stearidonic acids respectively. These two acids are then elongated to their [C.sub.20] isomers. These isomers are

then desaturated to their respective Δ^5 isomers. These Δ^5 fatty acids are used in prostaglandin formation.

CIS AND TRANS ISOMERS IN LIPIDS

Shani [3,4,5] studied the cis and trans isomers of jojoba oil and pointed out some differences in affinity of the two forms to silver ions, the naturally occurring cis form having somewhat more affinity. Trans isomers of lipid components are thermodynamically more stable and generally higher in melting point than the corresponding cis form. Wisniak [6] discusses different routes to achieve trans isomerization of jojoba oil and points out that partial hydrogenation and transisomerization of jojoba oil results in the formation of some trans fatty acid and fatty alcohol isomers.

Trans forms of unsaturated lipid materials can also be intentionally created through the use of a nitrous or selenium oxide catalyst and have commercial application as intermediates in various chemical reactions. Trans isomers of jojoba oil have been made (Jojoba Butter) by using heat in the presence of acidic bentonite clays [7]. Partial hydrogenation of vegetable oils and other lipid materials is, however, by far the most likely source of trans fatty acid isomers that subsequently enter the food and cosmetic chain of distribution.

Fully hydrogenated lipid materials contain neither cis nor trans fatty acid isomers. The double bonds of a fully hydrogenated lipid have been eliminated by completely "saturating" the molecule with hydrogen. This full hydrogenation reaction makes the carbon chain less active as a site for further reaction. A fully hydrogenated lipid material has a higher melting point and is more resistant to free radical formation (See Figure 3). Fully hydrogenated forms are also the most oxidatively stable of all possible chemical structures of lipids. Fully hydrogenated jojoba oil (melting point 68-70[degrees]C) contains neither cis nor trans isomers (there are no remaining double bonds in the molecule) and is frequently found as a component of lipsticks, mascara, eye shadow and other "wax matrix" type formulations.

Partial hydrogenation of lipid materials is routinely employed as a commercial means of incrementally increasing the oxidative stability of a lipid, increasing the melting point of the material and also as a means of altering the polarity of the material at the double bond site. "Brush hydrogenation" or "selective hydrogenation" or "selective saturation" are partial hydrogenation reactions often used as a means of "selectively" decreasing the polyunsaturated content of a lipid. These procedures create a higher melting fraction in the lipid, which can then be subsequently removed through a winterization or other fractionation process. "Brush hydrogenation" and "selective" hydrogenation or saturation reactions create unwanted trans isomers in lipids.

TRANS FATTY ACID ISOMERS IN COSMETICS

Figure 1. *cis* Double Bond

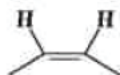
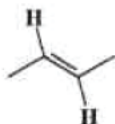


Figure 2. *trans* Double Bond



The CTFA List of Japanese Cosmetic Ingredients, 4th Edition (1999) lists seven "Partially Hydrogenated" product categories. These are Horse Oil, Jojoba Oil, Methyl Abietate, Palm Oil Fatty Acid, Perilla Oil, Squalene and Tallow Acid. Where INCI names for these lipids have been assigned in the USA, those INCI names do not include a "Partially Hydrogenated" category as in Japan. Formulators should be aware that "partially hydrogenated" and

"selectively hydrogenated/saturated" products containing trans isomers are sometimes offered to the trade under the INCI names of their fully hydrogenated analogs.

A search of the CTFA Dictionary for "partially hydrogenated" revealed two products; Pentahydrosqualene and Triethylene glycol hydrogenated rosinat. The CTFA Ingredient Dictionary also includes a listing for "Jojoba Butter," a transisomerized form of jojoba oil containing about 50% trans isomers.

ALTERNATIVES TO TRANS ISOMERS IN COSMETIC PRODUCTS

The challenge of cosmetic ingredient suppliers is therefore to provide manufacturers with oxidatively stable and affordable lipid based emollients that exhibit a broad range of melting points yet which contain no trans fatty isomers. Oil phase emollients with these desirable characteristics can be obtained without the formation of trans isomers through a process known as "interesterification." Rozenaal [8] discussed use of this interesterification process to modify the melting characteristics of triglycerides using various catalysts including enzymes. Another paper by Haumann [3] points out that the interesterification process may be a means of addressing the growing consumer concern for trans fatty acids.

Trans isomers of fatty acids that inhibit prostaglandin formation are rare in nature but can be found in partially (selectively) hydrogenated, brush hydrogenated or transisomerized lipid materials. Consumer awareness of the anti-nutritional effects of trans isomers in food products will lead to a heightened awareness of these compounds in cosmetics. Trans isomer presence in cosmetic ingredients is easy to detect, although often obscured due to improper, incomplete or misguided labeling by ingredient suppliers. Formulators should request certification from ingredient suppliers that confirm the absence of trans isomers.

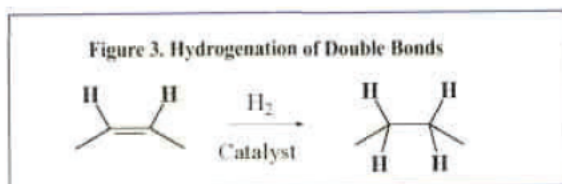
GLOSSARY OF TERMS

Lipids: Biomolecules insoluble in water that can be extracted from cells by high pressure or by organic solvents of low polarity such as hexane, ether, or chloroform. Examples of lipids are mono, di and triglycerides, wax esters, sebum, lecithin and phospholipids.

Fatty Acids: Generally, straight chain compounds, from three to twenty-four carbon atoms in chain length, having a terminal carboxyl group. These compounds make up the bulk of fats and oils and are important in skin nutrition.

Fatty Alcohols: Generally, straight chain compounds, from three to twenty-four carbon atoms in chain length, having a terminal hydroxyl group.

Trans Fatty Acids (Alcohols): Unsaturated fatty acids (alcohols) in which the hydrogens of the double bonds are on opposite sides of the molecule chain.



Cis Fatty Acids (Alcohols): Unsaturated fatty acids (alcohols) in which the hydrogens of the double bonds are on the same side of the molecule chain.

Hydrogenation: The addition of hydrogen atoms or molecules to unsaturated carbon chains (carbon chains with double bonds).

Saturation: Adding the maximum number of hydrogen atoms to an unsaturated bond. In the case of a double bond it is the addition of two hydrogen atoms, i.e., [H.sub.2]

Partial Hydrogenation: Incomplete addition of hydrogen to an unsaturated material leaving some double bonds not saturated, also known as "selective saturation" or "selective hydrogenation" or "brush hydrogenation." Partial,

brush or selective hydrogenates (saturates) contain unwanted trans isomers.

Interesterification: The catalyzed chemical reaction between two or more esters in which the acids and alcohols present are recombined in a random manner, also known as transesterification. This reaction does not alter the double bond geometry of unsaturated compounds, i.e., no trans isomers are formed as a result of interesterification reactions.

Transisomerization: The catalyzed chemical reaction converting natural cis double bonds to trans isomers. Transisomerization creates unwanted trans isomers.

James Brown is President of International Floratech, with headquarters in Arizona. Floratech manufactures botanical cosmetic ingredients. He may be contacted at jbrown@floratech.com. Robert Kleiman is the Technical Services Manager for International Flora Technologies, Ltd.

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- (2.) Rosenthal, M.D. and Doloresco, The Effects of trans Fatty Acids on Fatty [delta]5 Desaturation by Human Skin Fibroblasts, *Lipids*, vol. 19, (1984) pp. 869-874.

Acid	Structure	Source
trans-3-Hexadecenoic		Aster sp. Hopkins et. al, <i>Lipids</i> (1966)
trans-3-Octadecenoic		Grindelia ovalepis Kleiman et. al, <i>Lipids</i> (1966)
trans-3,cis-9,cis-12,trans-13-Octadecatetraenoic		Tecoma stans, Hopkins et. al. <i>J. Chem. Soc.</i> (1963)
cis-9,trans-11,trans-13-Octadecatetraenoic (alpha-Eleostearic)		Aleurites foetida (tung oil), Chronbie et. al. <i>J. Chem. Soc.</i> (1957)
9-hydroxy,trans-10,trans-12-Octadecadienoic (Dimorpheticolic)		Dimorphethesia tinctoria, Smith et. al. <i>J. Am Chem. Soc.</i> (1960)
4-keto,cis-9,trans-11,trans-13-Octadecatetraenoic (Lipoic)		Liscania rigida (oilseed oil), Brown, <i>Biochem. J.</i> (1933)
9-syn,trans-11-octadecenoic (Ximenesyn)		Ximenesia sp., Lighthelm et. al. <i>J. Chem. Soc.</i> (1952)

Table 1. Sources of Naturally Occurring Trans Fatty Acid Isomers

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Source Citation:

BROWN, JAMES, and ROBERT KLEIMAN. "Trans Isomers in Cosmetics." *Soap & Cosmetics* May 2001: 33.
Business Insights: Global. Web. 10 Nov. 2022.

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Document Number:

GALE|A75669667

