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Dr. Z Presents

Tech Notes

Triglycerides - Important Cosmetic Raw Materials

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Triglycerides, sometimes called oils, are natural products that are becoming more and more important to the cosmetic chemist. They are tri-esters of glycerin with three equivalents of organic acid.

Chemists are always interested in the composition and source of natural oils. The following is offered as a general overview of the topic. A book on the chemistry of triglycerides is available on the web free of charge1. Triglycerides can be classified into the following groups as shown:

Name	Source	CAS Number	Predominant Species
Class 1 - Animal derived products rich in carbon chain lengths below C-18			
Milk Fat	Cows Milk	8029-34-3	C16 triglyceride
Class 2 - Animal-derived products rich in C-18 unsaturated carbon chain lengths			
Tallow	Animal Fat	61789-13-7	C18:1 triglyceride
Japan Wax	Rhus succedanes	8001-13-6	C16 wax
Class 3 - Animal-derived products rich in carbon chain-lengths greater than C-			

18			
Beeswax	**Cera alba**	**8006-40-4**	**C26 wax**
Shellac Wax	**Shellac cera**	**97766-50-2**	**C30 wax**
Class 4 - Plant-derived products rich in carbon chain lengths below C-18			
Coconut Oil	**Cocus nucifera**	**8001-31-8**	**C12 triglyceride**
Babassu Oil	**Orbignya olefera**	**91078-32-1**	**C12 triglyceride**
Class 5 - Plant-derived products rich in C-18 unsaturated chain lengths			
Soybean Oil	**Glycerin soja**	**8001-22-7**	**C18:2 triglyceride**
Peanut Oil	**Arachis hypogaea**	**8002-03-07**	**C18:1 triglyceride**
Corn Oil	**Zea mays**	**8001-30-7**	**C18:1 triglyceride**
Sunflower Seed	**Helanthus annus**	**8001-21-6**	**C18:2 triglyceride**
Grape Seed Oil	**Vitis vinifera**	**8024-22-4**	**C18:3 triglyceride**
Safflower Oil	**Carthamus tinctorius**	**8001-23-9**	**C18:2 triglyceride**
Poppy Seed Oil	**Populus nigra**	**8002-11-7**	**C18:2 triglyceride**
Sweet Almond	**Prunnus amygdalus**	**8007-69-0**	**C18:1 triglyceride**
Oil	**dulcis**		
Hazelnut Oil	**Corylus americana**	**8007-69-0**	**C18:1 triglyceride**
Walnut Oil	**Juglans regia**	**8024-00-2**	**C18:2 triglyceride**
Olive Oil	**Olea europasa**	**8001-25-0**	**C18:1 triglyceride**
Avocado Oil	**Persea gratissima**	**8024-32-6**	**C18:1 triglyceride**
Sesame Oil	**Sesamum indicum**	**8008-74-0**	**C18:1 triglyceride**
Tall Oil	**Tallol**	**8002-26-4**	**C18:1 fatty acid**
Cottonseed Oil	**Gopssypium**	**8001-29-4**	**C18:2 triglyceride**
Palm Oil	**Elaesis guineensis**	**8002-75-3**	**C18:1 triglyceride**
Rice Bran Oil	**Oryza sativa**	**68553-81-1**	**C18:1 triglyceride**
Canola	**OilCanola**	**8002-13-9**	**C18:1 triglyceride**
Cocoa Butter	**Theobroma cao**	**8002-31-7**	**C18, C18:1 triglyceride**
Shea Butter Butyrospermum	**parkii**	**977026-99-5**	**C18 triglyceride**
Wheat Germ Oil	**Triticum vulgare**	**8006-95-9**	**C18:2 triglyceride**
Illipe Butter	**Cassia latifola**	**68424-60-2**	**C18 triglyceride**
Class 6 - Products rich in carbon chain lengths greater than C18			
Meadowfoam Seed Oil	**Limnanthes alba**	**153065-40-8**	**C20:1 triglyceride**
Rapeseed Oil	**Brassica capmestris**	**8002-13-9**	**C22:1 triglyceride**
Class 7 - Products having unusual carbon chain lengths or composition			
Borage Seed Oil	**Borago officinalis**	**8401201608**	**C18:3 (n=6) triglyceride**

Linseed Oil	**Linum usitatissimum**	**8001-26-1**	**C18:3 (cong) triglyceride**
Castor Oil	**Ricinus communis**	**8001-79-4**	**C18:1 OH triglyceride**
Veronia Oil	**Veronia galamensis**	**169360-96-7**	**C18 epoxy triglyceride**
Tung Oil	**Aleurites fordii**	**8001-20-5**	**C13:3 (cong) triglyceride**
Jojoba Oil	**Buxus chinensis**	**61789-91-1**	**C20 ester**
Candelilla Wax	**Euphorbia cera**	**8006-44-8**	**C32 hydrocarbon**
Ongokea Oil	**Ongokea gore**		**C18: acetylenic triglyceride**

Nature has provided a plethora of materials that are potentially useful in personal care applications. The type and source of natural raw materials is a major variable to be considered by the formulator in making new cosmetic products. The formulator needs to know some basic information about sources and chemistries of these raw materials to make informed decisions on product formulation. Not only performance, but also as importantly, cost and label copy is determined by the selection of oils and waxes, both per se and in surfactant molecules.

The process that allows for the transformation of a plant seed into clear, low odor oil suitable for cosmetic use is a process that we generally take for granted. The plant chosen for use as well as, the processing used, determines the properties of the oil.

The oils covered in this article are referred to as "vegetable oils." This differentiates them from "essential oils," which are often good-smelling oils that are steamed out of a variety of plant parts, including flowers, leaves, peels and some seeds. The essential oils are not triglycerides like the vegetable oils, but usually "isoprenoids." That is, they come from a different chemical pathway in plants. Plants store vegetable oils (triglycerides) as energy sources for seeds when they germinate.

Steam works well to extract essential oils like coriander oil, but not for triglyceride oils. Triglyceride and wax ester oils can be squeezed out of seeds using a turning screw that presses the mashed up seed against a metal barrel with slits in the side. The oil and some fine particles squeeze out the narrow slits. This operation would be called an oil expeller or seed oil press. The oil from the seed oil press can be filtered and called "virgin" oil, especially if it isn't heated up to get more oil out. The oil from the seed oil press can also be called crude oil. Alternatively, oil can be dissolved in solvent, followed by evaporating of the solvent leaving the extracted oil.

Often, seeds are flaked to increase surface area. The seeds are processed into thin flakes before pressing or solvent extraction. The flaking improves oil yield by breaking open the small oil pockets in the seeds. Sometimes the seeds are heated before flaking so that the proteins in the seed won't break down the oil or other things in the seed. The preheating is also called preconditioning. The oil comes out more easily if it is hot, but too much heat damages the oil quality.

Sometimes the seeds are crushed and formed into pieces called "collets" that have lots of holes or openings. This step is also done before solvent extraction to make the oil to flow out easier. Solvent-extracted-oil with some

solvent still in it is called the "miscella."

This crude oil is usually enough for chemical uses, usually. A well-filtered "virgin" oil can be kept cold to remove any solid waxes that might crystallize out in a process called "winterization."

Many cosmetics applications require cold-pressed, virgin oil. On the other hand, some seeds are too low in oil to economically remove the oil by pressing. In any case, once you have the crude oil, you can move onto refining. Refining is done by filtering the oil through clay or silica, which can remove color. In an operation called "degumming," alkali in water is added to the oil and some ingredients, especially fatty acids and one called "phospholipids" are solubilized or precipitated or are filtered out. Finally, steam can be passed through the oil to remove odor in an operation called deodorization. This step also breaks down oxygen attached to the oil, which might lower oil quality. Hopefully, after all of this refining the oil is light in color, has no odor, no oxygen breakdown products and no solid wax. The amount of oil you have left after refining is related to the amount of crude oil you started with or to the amount of oil in the seed extracted by each step in the process.

The oils that are commonly used in cosmetic products are complex mixtures of different triglycerides, but also contain various other components that are useful. For example, olive oil can be processed to contain highly desirable tocopherols. Solvent extraction or steam distillation would remove much of this material. If the oil was in the formulation for the benefit derived from the tocopherols, the potential variations in the processing could have dramatic consequences. The winterizing of oils, that is cooling and filtration of solids from the liquid, results in a loss of the higher molecular weight fractions. Many times, it is exactly these fractions that provide the unique skin feel or conditioning to the product. It should be clear that the different processes used in the preparation of an oil may be critical to functionality.

Methyl Esters

Triglycerides may be easily turned into methyl esters by reaction with methanol and catalyst. Base catalysts are preferred. As the reaction proceeds, the reaction mixture turns hazy as glycerin is liberated. Once complete, the excess methanol is distilled off, glycerin removed from the bottom after it settles and the methyl ester is distilled into its fractions.

The methyl ester formed by the reaction, if not distilled, is still referred to by the oil name (for example methyl cocoate). However, once fractionated, the material is named by carbon distribution. Methyl cocoate is fractionated into methyl laurate, methyl myristate and so on. The triglyceride source is lost in the name of the methyl ester. The names for the common alkyl groups are given below. Distillation is a major operation used to fractionate the methyl ester mixture gotten from oils into specific defined methyl esters having the desired alkyl groups.

Fatty Acids

Fatty acids are also available that have specific "cuts". They include acids having a wide distribution, like coco fatty acid (having essentially the same distribution as the oil). They also include very specific cuts having a composition of a single fatty acid. One of the most confusing aspects of dealing with fatty acids is the nomenclature.

Commonly Used Fatty Acid Nomenclature:

Designation	Name	Formula
C6	Caproic Acid	C6H12O2
C8	Caprylic Acid	C8H16O2
C10	Capric Acid	C10H20O2
C12	Lauric Acid	C12H24O2
C12:1	Lauroleic acid	C12H22O2
C14	Myristic acid	C14H28O2
C14:1	Myristoleic acid	C14H26O2
C16	Palmitic acid	C16H32O2
C16:1	Palmitoleic acid	C16H30O2
C18	Stearic acid	C18H36O2
C18:1	Oleic acid	C18H34O2
C18:2	Linoleic acid	C18H32O2
C18:3	Linolenic acid	C18H30O2
C20	Arachidic acid	C20H40O2
C20:1	Gadoleic acid	C20H38O2
C22	Behenic acid	C22H44O2
C22:1	Erucic acid	C22H42O2
C22:2	Clupanodinic acid	C22H40O2
C24	Lignoceric acid	C24H48O2
C26	Cerotic acid	C26H52O2
C28	Montanic acid	C28H56O2
C30	Myricic acid	C30H60O2
C32	Lacceroic acid	C32H64O2
C34	Geddic acid	C34H68O2

There is a wide-range of products that are produced by utilizing the various fatty acids and methyl esters made using these processes.

References:

1. www.zenitech.com Primary Ingredients by O'Lenick, Anthony J., Steinberg, David and Klein Kenneth, 1998.
2. O'Lenick, Anthony J., Surfactants Chemistry and Properties 1999, Allured Publishing Corporation p. 13-15.