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DHA (Dihydroxyacetone)

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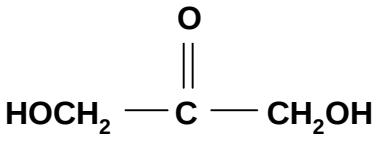
A. Technical Data Sheet

INCI Name: Dihydroxyacetone
Product Code: SC-8808
Chemical Name: 1,3-dihydroxy-2-propanone
CAS No.: 62147-49-3(Dimer); 96-26-4(Monomer)
EINECS No.: 202-494-5
Molecular Formula: $C_3H_6O_3$



Biological Activity
when applied to the skin causes a chemical reaction with amino acids in the surface cells of the skin producing a darkening effect. DHA does not damage skin as it only affects the outermost cells of the epidermis (stratum corneum).

Cosmetic Application
Sunless tanners. To date, it is the only active ingredient approved by the US Food & Drug Administration (FDA) for sunless tanning.

Use level: 2.5 to 10% or more (mostly 3-5%)

Main Specification:

Appearance:	**white crystalline powder**
Purity:	**≥ 98%**

Package: 25kg carton lined a PE bag.

Storage: Hygroscopic. Regrigerate at<6℃,in Original sealed containers.

[Caution]
Formulation should be done at a temperature below 40℃ and a pH between 4 and 6.

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B. Introduction

Dihydroxyacetone (DHA) is currently the most popular way of gaining a tan-like appearance without sun exposure as it carries less health risks than any of the other available methods. To date, it is the only active ingredient approved by the US Food & Drug Administration (FDA) for sunless tanning.
SpecChem has developed a biotechnological process to produce this active, which consists of a bioconversion of glycerol.

Natural source

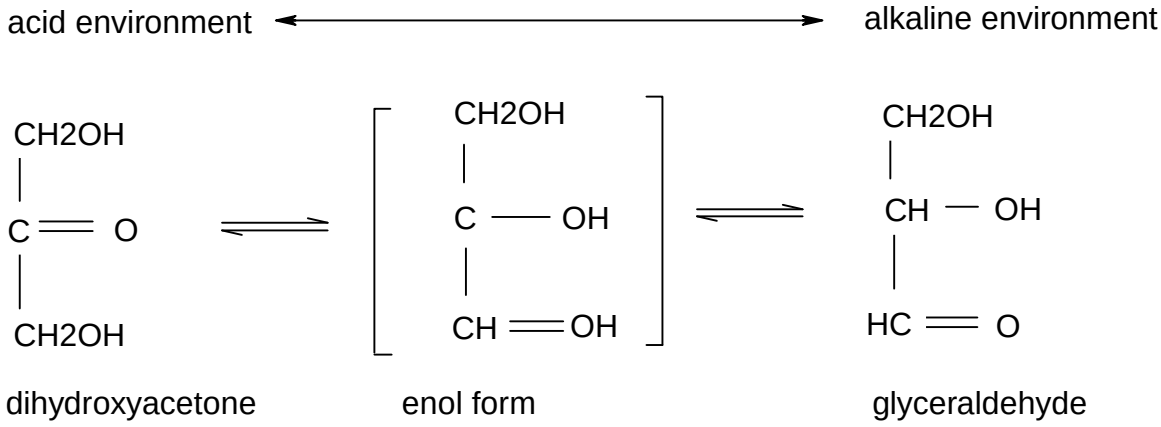
DHA and glyceraldehydes, present in equilibrium, occur in the form of their phosphoric acid esters in carbohydrate metabolism. The breakdown of fructose-1,6-dihydroxyacetone phosphate and glyceraldehydes-3-phosphate. Both substances form a reversible equilibrium system. The aldehyde reacts further, forming pyruvate which enters the citric acid cycle. This chain of reaction is also known as "Embden –Meyerhof degradation".

Activity

DHA interacts with the components of the upper layer of the epidermis (Maillard reaction). The brown colouring appears after a reaction time of at least 2 hours; it can not be washed of, but fades as the upper layers of the epidermis are shed.

Behaviour and Stability in aqueous solution

In aqueous solution dihydroxyacetone occurs as a monomer which can gradually tautomerize into glyceraldehydes. The equilibrium is shifted according to the pH of the solution.



Under alkaline conditions, stating from glyceraldehydes, various isomerization and condensation reactions occur which ultimately lead to the formation of brown- colored oligomers. Glyceraldehyde itself can also play a role in theMailard reaction chain.

When referring to the stability of DHA, one must distinguish between DHA content, pH value and the occurrence of by-procducts such as formaldehyde and organic acids present at ppm levels.

DHA content can be dramatically reduced by incorrect storage conditions or processing at too high temperatures. Via decomposition or rearrangement reactions, aldehydes and ketones e.g. methyl-glyoxal can be formed, some of which nevertheless themselves have a tanning effect.

The pH value of DHA solution drops over time to ca. pH 3 due to the formation of organic acids.

Depending on temperature and storage duration, by-products such as formaldehyde and organic acids, e.g. formic acid are produced. These are responsible for reduction in pH value and in part also for the occurrence of an acidic smell.

Toxicological and Dermatological Studies

LD_{50}	oral rat	> 16.0g/kg bodyweight
	i.p.rat	> 6.4 g/kg bodyweight

Dihydroxyacetone was tolerated well by rabbits in acute skin and mucous membrane tolerance tests (1).
Dihydroxyacetone reacts with the norny layer of the skin and does not penetrate into the deeper skin layer (2).

(1) Study of the acute toxicity in rats after oral administration and intraperitoneal injection and of primary irritation on skin and mucus membranes in rabbits.
(2) Absorption of reactivity of 14C-Dihydroxyacetone(DHA) through the skin after single dose dermal application of 50mg to six healthy volunteers.

Application

Dihydroxyacetone can be used in various cosmetic formulations. Emulsions of the O/W and W/O types are appropriate for this purpose as well as aqueous lotions and gels.

The content of dihydroxyacetone in tanning products depends on the desired browning intensity on the skin and is normally in the range ca. 2 to 5%. Depending on the type of the formulation and skin type a tanning effect appears on the skin about 2 to 3 hours after use.

During product storage, the pH of a DHA-containing formulation will drift over time to ca.3-4 at which DHA is particularly stable.

Use of buffers to maintain the pH of a formulation above 4.5 is not recommended. The pH of the formulation may be adjusted to approximately 3-4 by using citric acid. Phosphate buffers are not recommended. At pH values above 7, brown-coloured compounds are produced via

isomeration and condensation reactions and product effectiveness is reduced.

When developing self-tanning products a few general guidelines must be followed in order to ensure end product stability.

The following factors have a negative effect on the stability and effectiveness of dihydroxyacetone:

1. **heat**
2. **compounds containing nitrogen**
3. **perfume oils/extracts**
4. **microorganisms**
5. **oxygen/oxidizing agents**

For the above reasons the following notes and precautions should be carefully taken into consideration when new formulations containing dihydroxyacetone are developed.

As a raw material dihydroxyacetone should be stored in tightly closed containers in a cool place(< 6℃). Furthermore, products containing dihydroxyacetone should be sold in an opaque, resealabel package. Heating dihydroxyacetone to above 40 ℃ for long periods of time should be avoided. During manufacture involving heating processes, as in the case of emulsions, dihydroxyacetone should not be added until the formulation has been cooled down to below 40℃.

If this not possible, the formulation must be cooled as rapidly as possible to below 40℃ to keep thermal stress on DHA to a minimum.

A further concern is the susceptibility of DHA to microbial attack in aqueous solutions. For this reason preservation of the final product and also hygienically clean manufacturing and packing procedures are particularly important.

Apart from these general recommendations one should also look more specifically at the final formulation and its individual components. The reactivity of DHA with several ingredients typically used in cosmetics can lead to gradual breakdown of the active substance and thus to a loss of compounds should be included in the final formulation. Collagen, urea derivatives, amino acids, proteins etc. should be avoided.

Discolouration is also observed in formulations containing polyacrylic acid derivatives. Cellulose ethers and xanthan gum are recommended gallants.

It must be noted that a tan achieved with DHA alone does not offer the sun protection resulting from natural melanin production during sunbathing. It is, however, possible to combine DHA

with non-nitrogen-containing UV filters to achieve a product with additional sun protection effect.

The choice of perfumes which are compatible with DHA also plays an important role.

Product Properties

	Monomer form in solution	Dimeric forms solid
Empirical formula	$C_3H_8O_3$	$C_6H_{12}O_6$
Molar	90.08g/mol	180.16 g/mol
Solubility in water	readily soluble	converted in water to the monomer form
Solubility in 70% form	readily soluble	converted in ethanol to the monomer
Melting Point	68-71℃	71-82℃
Storage	store in a cool, dry place (at < 6℃)	
Shelf life	min. 1 year	

Specification(Conforms to the requirements of the USP)

Appearance	White to off-white, crystalline powder; faint characteristic odour; slightly hygroscopic.
Assay	98.0-102%
Identity	IR spectrum conforms
pH value(5% in water)	4.0-6.0
Heavy metals(as Pb)	≤ 0.001%
Arsenic(As)	≤ 0.0003%
Iron(Fe)	≤ 0.002%
Protein(colorimetric as BSA)	≤ 0.01%
Glycerol(TLC)	≤ 0.5%
TLC examination (Chromatographic purity)	conforms
Sulfate ash	≤ 0.1%
Water(Karl.Fischer)	≤ 0.2%
Microbial Purity(USP)	≤ 100 CFU/g, no pathogens

Storage Conditions/Packaging

Keep dry and cool at 2 – 8°C. Slightly hygroscopic. Slightly hygroscopic.
Allow to reach room temperature before opening drum.

C. Formulation

1. Self Tan Cream containing DHA

Phase	No.	Product Name / INCIName	%	Supplier
A	1	Tego® Care 150	8.0	Degussa
	2	Cetearyl Alcohol	1.0	Cognis
	3	Eutanol G	2.0	Cognis
	4	Mineral Oil (26#)	5.0	
	5	MYRITOL 318	2.0	Cognis
	6	CETIOL CC	2.0	Cognis
	7	DC200	0.5	Dow Corning
	8	α- Bisabolol,	0.2	SC
	9	BHT	0.05	
	10	Propylparaben	0.1	
B	1	Glycerin	3.0	
	2	Poria Cocos Root Extract（1%）	5.0	SC
	3	Methylparaben	0.2	
	4	NMF-50(Trimethylglycine)	1.0	SC
	5	Deionized Water	To 100	
C	1	IS-45	0.4	ISP
	2	Fragrance	qs.	
D	1	DHA	5.0	SC
	2	Deionized Water	10.0	

Procedure:

1. Add various raw materials in Phase A (Oil Phase) into the vessel, heat and stir to dissolve, control the temperature around 80±2℃.
2. Heat and stir raw materials in Phase B (Water Phase) to completely dissolve. Stop heat when temperature reach to around 90℃. Keep temperature at 80℃ prior to emulsification.
3. Suck Oil Phase into emulsification vessel, and then under continuous stirring suck Water Phase into the vessel. Emulsify for 15 min.
4. Cool the resulting mixture to 48℃, increase the speed of stirrer equipped with plough blade, add Phase C, continue stir.
5. Cool to below 40℃, add Phase D, stir well.

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2. Self Tan Milk containing DHA

Phase	No.	Product Name / INCI Name	%	Supplier
A	1	GP200	2.0	Croda
	2	Cetearyl Alcohol	0.5	Cognis
	3	Glyceryl Stearate	0.5	Cognis
	4	Mineral Oil	1.0	
	5	Isopropyl Myristate	1.0	Cognis
	6	CETIOL CC	2.0	Cognis
	7	DC-200	0.5	Dow Corning
	8	Ethylhexyl Ethylhexanoate	1.0	Symrise
	9	α- Bisabolol,	0.2	SC
	10	BHT	0.05	
	11	Propylparaben	0.1	
B	1	Glycerin	4.0	
	2	Xanthan Gum	0.05	SC
	3	Poria Cocos Root Extract（1%）	5.0	SC
	4	Allantion	0.2	
	5	Methylparaben	0.2	
	6	HR-S_1 (potassium cetyl phosphate	0.7	
	7	NMF-50(Trimethylglycine)	1.0	SC
	8	Deionized Water	To 100	
C	1	IS-45	0.4	ISP
	2	Fragrance	qs.	
D	1	DHA	5.0	SC
	2	Deionized Water	12.0	

Procedure

1. Heat under stirring Phase A (Oil Phase) to dissolve, control temperature at 80±2℃.
2. Pre-mix 1 and 2 in Phase B (Water Phase) and disperse well. Add water, then heat with stirring to completely dissolving. Stop heat when temperature reach around 90℃. Keep temperature at around 80℃ prior to emulsification.
3. Firstly such Oil phase into emulsification vessel, and under continuous stirring suck water phase into the vessel, emulsify for 15 minutes.

4. **Cool the resulting mixture to 48℃, increase the speed of stirrer equipped with plough blade, add Phase C, continue stir.**
5. **Cool to below 40℃, add Phase D, stir well.**

D. Other uses

1. Intermediate for synthesis of various organic compounds.

2. Reduction of Carcass Fat in Swine with Dietary Addition of Dihydroxyacetone and Pyruvate

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ABSTRACT

Swine weighing 80 to 85 kg were fed a basal corn-soybean meal diet plus a mixture of dihydroxyacetone and pyruvate (3:1) (triose) or Polycose| (control), a glucose polymer, as 3.85% of calories (4% of the diet). Twenty-four pigs were pair-fed the triose mixture or control diet for 28 d in litter-mate pairs of the same sex. Weight gain and feed consumption were recorded and carcasses were evaluated for fat and muscle accretion. The right rear leg and rear one-third of the right loin were skinned, deboned, ground and analyzed for protein, fat, moisture and ash content. Average backfat depth and backfat depth at the first, last and 10th rib were reduced by 12, 15, 14 and 12% (P < .01), respectively, in lriose-fed pigs. Loin eye area and untrimmed lean cuts were not altered by diet, but percentage trimmed lean cuts was higher (P < .02) in triose-fed pigs (57.6 vs 55.3%). Leg and loin tissue samples from pigs fed the triose mixture had a lower (P < .01) percentage of fat and a corresponding increased (P < .01) percentage of protein. Organ weights and the blood biochemical profile were not altered by triose feeding. Liver function tests were not altered in animals consuming the trioses, except for an 18% decrease (P < .05) in serum glutamic pyruvic transaminase. Ingestion of dihydroxyacetone and pyruvate will reduce body fat in limit-fed swine without reducing muscle protein deposition.

(Key Words: Swine, Carcass Composition, Trioses, Pyruvate.)

J. Anita. Sci. 1989. 67:1272--1278