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BATH OIL COMPOSITION CONTAINING OCTYL DODECANOATE

Edward J. Conklin, Forest Park, and Leo F. Judge, Jr.,
Cincinnati, Ohio, assignors to The Procter & Gamble
Company, Cincinnati, Ohio, a corporation of Ohio
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The present invention relates to a bath oil of novel composition. More particularly, this invention relates to a bath oil, suitable for cosmetic and therapeutic purposes, which is comprised of particular fatty esters and mineral oil, and which, in its preferred embodiment, contains lower molecular weight alcohols and nonionic surfactants.

The beneficial effect of oil on the skin is well known. Dermatologists have long extolled the merits of oil in protecting and reconditioning skin, especially dry skin.

In this connection, dry, pruritic, scaly and pediatric dermatoses all appear to be caused, at least to some degree, by lack of water in the outer skin layer, the stratum corneum. Skin lipids play a significant role in keeping the skin soft and flexible by preventing water loss from the stratum corneum. The cells of this outer layer are highly hydrophilic and will swell considerably when immersed in water or when water is supplied by internal means through the sweat glands. However, when the humidity is low, water present in the skin may be lost at a higher rate than it can be replaced internally. This water loss, in turn, tends to cause skin dryness and related problems. The purpose of the bath oil is to augment the skin lipids by forming a protective film on the skin. The bath oil thus assists in keeping moisture in the stratum corneum and, accordingly, tends to keep the skin soft, silky and smooth without the danger of chapping.

In the first attempts to use a bath oil, oil was simply poured into the water and an oil film was formed on the surface of the water. As the bather stepped into and out of the bath water, his skin was coated with the oil floating on the water. This method of application left the skin with an excessively greasy feeling and was found to leave a visible coating of oil on the skin, some of which rubbed off on garments. The oil coating was also visible as a bathtub ring. Therapeutically, this method did accomplish the results of coating the skin to retard evaporation of moisture, but the problems it raised prevented wide consumer acceptance.

Improved bath oil compositions were later prepared by mixing with a mineral oil a compound such as isopropyl myristate, or isopropyl palmitate. Because of the addition of these esters, the resulting surface tension in the oil and ester mixture was less than that of the oil alone. Accordingly, the thickness of the molecular layer on the surface of the water was decreased. Reduction of the thickness of the bath oil layer alleviates the excessively greasy feeling caused by absorption of excess oil on the skin, yet allows deposit of sufficient emollient to keep the skin soft, smooth and flexible. This ester also tends to act as an extender or spreading agent. These specific esters, however, failed to satisfactorily solve the problems of the formation of the unsightly oil ring in the bathtub.

It has now been discovered that an improved bath oil composition can be prepared which not only renders the skin as soft and pliable as previous products but which also aids in eliminating the troublesome problem of bathtub rings.

Accordingly, it is a primary object of the present invention to provide an improved bath oil composition which has valuable emolliency and therapeutic properties. Another object of this invention is to provide a bath oil

composition which retards the formation of the unsightly bathtub ring.

Yet a further object of this invention is to provide a bath oil composition containing as an essential ingredient, an emolliency and therapeutic agent which will effectively coat the skin to prevent water loss from the stratum corneum and, at the same time, give the skin a smooth, silky feeling.

Still further objects and the entire scope of applicability of the present invention will become apparent from the detailed description given hereinafter; it should be understood, however, that the detailed description and specific examples, while indicating preferred embodiments of the invention, are given by way of illustration only since various changes and modifications within the spirit and scope of the invention will become apparent to those skilled in the art from this detailed description.

It has now been discovered that the foregoing objects of the present invention are attained with a novel bath oil composition which is a clear, non-aqueous liquid consisting essentially of from about 20% to about 80% of an ester having moieties containing from about 8 to about 14 carbon atoms, from about 20% to about 80% of a mineral oil, from 0% to about 30% of an alcohol containing from 2 to 10 carbon atoms and from about 0% to about 10% of a synthetic nonionic surface active agent.

The esters utilized in the bath oil compositions herein described have moieties containing from about 8 to about 14 carbon atoms. More particularly, the esters of these compositions can conveniently be described as the esters of branched or straight chain saturated aliphatic alcohols having from about 8 to about 14 carbon atoms and preferably from 8 to 12 carbon atoms and branched or straight chain aliphatic fatty acids having from about 8 to about 14 carbon atoms and preferably from 8 to 12 carbon atoms. Although optimally comprised of esters having from about 8 to about 14 carbon atoms in each moiety, the composition can tolerate up to about 15% of the total ester mixture of alcohols or fatty acids which deviate from the delineated carbon atom limits by not more than 4 carbon atoms.

It was surprising to discover that bath oil compositions containing these fatty esters fulfilled the objectives of this invention. Heretofore, it had been thought that only those esters which were of the isopropyl myristate and isopropyl palmitate variety could be used in combination with other bath oil ingredients. That is, it was heretofore considered essential to employ esters which structurally had a long acyl moiety and a very short alkyl chain. It was also suspected that esters having a more symmetrical configuration would not possess the property of being compatible with the essential bath oils.

It has been unexpectedly found, however, that these esters are compatible with the other bath oil ingredients. Additionally, valuable therapeutic and emollient effects are attributed to these esters. They render a markedly smoother and silkier feeling to the skin than do the esters of the isopropyl myristate type. They also contribute substantially to alleviating the problem of bathtub ring.

Examples of specific esters suitable for use in this invention are 2-ethylhexyl dodecanoate, 2-ethylhexyl octanoate, octyl octanoate, octyl dodecanoate, dodecyl dodecanoate, decyl decanoate, decyl octanoate and octyl 1,1-dimethyldodecanoate.

The esters of this invention can be utilized alone or they can be utilized in admixture with each other in any proportions. In fact, as a preferred embodiment of the present invention, esters derived from natural sources are utilized in this bath oil composition.

One of these preferred ester ingredients, characterized in column 1 of Table I, can be prepared by the alcoholysis of a mixture of light cut coconut methyl esters

with a mixture of light cut coconut alcohols. It is to be understood that light cut coconut, in this context, refers to a coconut fraction containing the following approximate distribution of carbon chain lengths: 4% C₆, 60% C₈, 35% C₁₀ and 1% C₁₂. Another preferred ester component characterized in column 2 of Table I, and referred to hereinafter as essentially octyl dodecanoate, can be prepared in the same manner by utilizing a mixture of middle cut coconut methyl esters, i.e., a fraction containing the following approximate distribution of carbon chain lengths: 1% C₁₀, 68% C₁₂, 24% C₁₄, and 7% C₁₆, and a mixture of light cut coconut alcohols as identified above.

An analysis of these coconut cut esters follows.

TABLE I.—ANALYSIS OF ESTERS

	Col. 1 Essentially octyl octanoate	Col. 2 Essentially octyl dodec- anoate	Col. 3 Essentially dodecyl dodecanoate
Molecular weight.....	273	318	388
Saponification value.....	203	176	145
Acid value.....	0.05	0.02	0.5
Iodine value.....	0.09	0.1	0.3
Hydroxyl value.....	1.03	1.03	2.0
Melting point (° C.).....	-13	9	29
Specific gravity (25°/25° C.)....	0.856	0.856	0.850

The liquid esters of the present invention, such as octyl octanoate, octyl dodecanoate, and 2-ethylhexyl dodecanoate, are clear, mobile liquids with high boiling points and high flash points. They are very soluble in common organic solvents but insoluble in water. Dodecyl dodecanoate is a solid and is hard and wax-like with a more limited solubility in organic and inorganic solvents. Additionally, all of the esters of this invention are nearly odorless and colorless, which in conjunction with their low potential for irritation and oily consistency make them excellent bath oil adjuvants.

The esters of this invention can advantageously be prepared by the process known as alcoholysis. During this reaction, the alcohol moiety of an ester of an organic acid is replaced by that of another alcohol. Such methyl esters as those of octanoic, decanoic or dodecanoic acids can, accordingly, be permitted to react with alcohols containing from about 8 to about 14 carbon atoms to obtain the esters of this invention. Catalysts suitable for use in this reaction are strong bases such as the aluminum alkoxide of the free alcohol, sodium methoxide or acids such as sulfuric or hydrochloric acid. Other methods suitable for preparation of these esters are described in Kelley, Organic Chemistry, 2nd ed. (1957), at pp. 167-169. It is not intended that the esters of this novel composition be limited to any particular source or method of preparation; the only restriction on these esters is embodied in the description of the moieties.

According to the present invention, these esters should comprise from about 20% to about 80% by weight of the total bath oil composition. In the preferred embodiment of this invention, however, the esters should be used at a level of from about 40% to about 75% by weight of the total composition. If these limitations are not met, optimum therapeutic, emollient and cosmetic effects are not attained. In addition, the problem of bathtub rings is averted.

Oils suitable for conjoint use with the hereinbefore disclosed esters may be selected from a large class of materials. The preferred oil is mineral oil, as it appears to be absorbed in greater quantities on the skin and gives longer lasting comfort and smoothness.

Mineral oil is a colorless, transparent, oily liquid that is obtained from crude petroleum by refining. Essentially all of the unsaturated and aromatic hydrocarbons and other impurities are removed, and the resulting oil product is clear and water-white or nearly water-white. The United States Pharmacopoeia defines two types of white mineral oil, or liquid petrolatum. One type, which has a

kinematic viscosity of not more than 37 centistokes at 37.8° C. (100° F.), is termed light; the other, with a kinematic viscosity of not less than 38.1 centistokes, is termed heavy. Since viscosity is usually expressed in Saybolt seconds, this distinction between grades should be understood as follows: A white mineral oil that has a Saybolt viscosity of not more than 172 at 100° F. is referred to as light white mineral oil, while one that has a Saybolt viscosity of not less than 177 is termed heavy white mineral oil. While either of these mineral oils or mixtures thereof may advantageously be utilized in this composition, as an especially preferred embodiment herein, light white mineral oil is utilized herein.

When suitable standards for mildness, toxicity and odor are followed, other oils can be substituted for the mineral oil. Examples of other oils which can be used beneficially in the composition of this invention are vegetable oils such as sesame oil, cottonseed oil or corn oil. Other acceptable vegetable oils are sweet almond oil, olive oil, wheat germ oil, rice bran oil and peanut oil. Animal oils that may be utilized in this bath oil composition are lanolin, neat's foot oil, bone oil, sperm oil, cod liver oil, and the like.

All of these oils may be used either alone or in conjunction with each other. They may be mixed in any suitable ratio and may be specifically formulated for particular uses.

The oil component should be used at a level of from about 20% to about 80% by weight of the total composition. As a preferred embodiment of this invention, the oil component is added in amounts of from about 25% to about 60% by weight of the total composition. In the preferred range, the product has little greasy feeling and is optimally suited for retarding moisture loss from the skin.

According to a preferred embodiment of this invention, a nonionic surface active agent is present in this composition. The nonionic surfactants which are broadly suitable for use in this invention may be defined as those surfactants which do not ionize in water solution.

For example, a well known class of nonionic surfactants is made available on the market under the trade name of "Pluronic." These compounds are formed by condensing ethylene oxide with a hydrophobic base formed by the condensation of propylene oxide with propylene glycol. The hydrophobic portion of the molecule which, of course, exhibits water insolubility has a molecular weight of from about 1100 to 2500. The addition of polyoxyethylene radicals to this hydrophobic portion tends to increase the water solubility of the molecule as a whole, and the liquid character of the product is retained up to the point where polyoxyethylene content is about 50% of the total weight of the condensation product.

Other suitable nonionic surfactants include:

(1) The polyethylene oxide condensates of alkylphenols, e.g., the condensation products of alkylphenols or dialkylphenols wherein the alkyl group contains from about 6 to 12 carbon atoms in either a straight chain or branched chain configuration, with ethylene oxide, the said ethylene oxide being present in amounts equal to 5 to 25 moles of ethylene oxide per mole of alkylphenol. The alkyl substituent in such compounds may be derived from polymerized propylene, diisobutylene, n-octene, or n-nonene, for example.

(2) The condensation product of aliphatic alcohols having from 8 to 18 carbon atoms, in either straight chain or branched chain configuration, with about 3 to 50 moles of ethylene oxide, e.g., a coconut alcohol-ethylene oxide condensate having from 10 to 30 moles of ethylene oxide per mole of coconut alcohol, the coconut alcohol fraction having from 10 to 14 carbon atoms.

(3) Those derived from the condensation of ethylene oxide with the product resulting from the reaction of propylene oxide and ethylenediamine. For example, compounds containing from about 40% to about 80% poly-

were added in the order listed below. Between each addition, the product was stirred to insure uniformity of the final bath oil. Since a major factor in consumer acceptance of this type of product is odor, and in view of the high dilution of the product in usage, relatively high levels of perfume are used in these formulations.

EXAMPLE I

The following clear formulation of this invention was compared with a commercially successful bath oil which contained isopropylmyristate.

	Percent by weight
Essentially octyl dodecanoate ¹	50
Light white mineral oil (graded by United States Pharmacopoeia)	35
Condensation product of nonyl phenol with 9.5 moles of ethylene oxide	5
Isopropyl alcohol	7
Perfume and color	3

¹ The octyl dodecanoate component was prepared by the alcoholysis of a mixture of middle cut coconut methyl ethers with a mixture of light cut coconut alcohols. The middle cut coconut fraction contained the following distribution of carbon chain lengths: 1% C₁₀, 68% C₁₂, 24% C₁₄ and 7% C₁₆. The light cut fraction contained 4% C₈, 60% C₈, 35% C₁₀ and 1% C₁₂.

These two formulations were compared in home use tests. Panelists used these products over a period of time and were then asked to register their preferences. They were not informed of the compositions being tested. There was a decided overall preference for the clear composition of this invention.

EXAMPLE II

The following bath oil compositions were prepared. In all the formulations listed below, the product was a clear, homogenous, liquid mixture which, when applied in the normal bathtub manner to the skin, left it feeling smooth, soft and silky. The formation of the bathtub ring was substantially retarded during use of several formulations by using the dispersants and emulsifiers as hereinbefore described.

In the following formulations, the esters, octyl octanoate, octyl dodecanoate, dodecyl octanoate and dodecyl dodecanoate, were prepared from coconut fractions. The octyl octanoate ester is the reaction product of light cut coconut methyl esters and light cut coconut alcohols. The octyl dodecanoate ester is the reaction product of middle cut coconut methyl esters and light cut coconut alcohols while the dodecyl octanoate ester is the reaction product of light cut coconut methyl esters and middle cut coconut alcohols. Middle cut coconut methyl esters and middle cut coconut alcohols were utilized in preparing the dodecyl dodecanoate. The terms "light" and "middle" have been hereinbefore defined.

Formulation 1:	Parts by weight
Octyl dodecanoate	50
Light white mineral oil (graded by United States Pharmacopoeia)	47
Perfume and color	3
Formulation 2:	
Octyl octanoate	40
Heavy white mineral oil (U.S.P. Grade)	60
Formulation 3:	
Octyl dodecanoate	50
Light white mineral oil (U.S.P. Grade)	37
The condensation product of nonyl phenol with about 9.5 moles of ethylene oxide	6
Ethanol	7
Formulation 4:	
2-ethylhexyl dodecanoate	52
Lanolin	29
The condensation product of sorbitan dodecanoate with about 20 moles of ethylene oxide	8
1,2-propanediol	11

Formulation 5:	Parts by weight
Octyl dodecanoate	43
Light white mineral oil (U.S.P. Grade)	47
The condensation product of a mixture of isomeric linear secondary alcohols containing from 11 to 15 carbon atoms with about 9 moles of ethylene oxide	5
Ethanol	5
Formulation 6:	
Octyl dodecanoate	60
Light white mineral oil (U.S.P. Grade)	30
Benzyl alcohol	10
Formulation 7:	
Dodecyl octanoate	40
Light white mineral oil (U.S.P. Grade)	50
Hexanol	10
Formulation 8:	
Octyl dodecanoate	42
Heavy white mineral oil (U.S.P. Grade)	24
Light white mineral oil (U.S.P. Grade)	24
N,N-diethanoldodecanamide	7
Perfume, color	3
Formulation 9:	
Octyl dodecanoate	46
Light white mineral oil (U.S.P. Grade)	35
The condensation product of nonyl phenol with 9.5 moles of ethylene oxide	7
Ethanol	6
N,N-diethanoldodecanamide	6
Formulation 10:	
Octyl dodecanoate	60
Light white mineral oil (U.S.P. Grade)	35
N-ethanol octanamide	5
Formulation 11:	
2-ethylhexyl dodecanoate	60
Light white mineral oil (U.S.P. Grade)	35
Octanamide	5
Formulation 12:	
Octyl dodecanoate	50
Light white mineral oil (U.S.P. Grade)	41
N-ethanol octanamide	4
Ethanol	5
Formulation 13:	
Dodecyl octanoate	45
Light white mineral oil (U.S.P. Grade)	22
Heavy white mineral oil (U.S.P. Grade)	23
Tetradecanamide	5
2-propanol	5
Formulation 14:	
Octyl octanoate	50
Light white mineral oil (U.S.P. Grade)	40
N,N-diethanoldodecanamide	5
Butanol	5
Formulation 15:	
Octyl dodecanoate	46
Light white mineral oil (U.S.P. Grade)	35
The condensation product of nonyl phenol with 9.5 moles of ethylene oxide	7
Ethanol	6
N-ethanoldodecanamide	6
Formulation 16:	
Dodecyl octanoate	46
Light white mineral oil (U.S.P. Grade)	36
The condensation product of sorbitan dodecanoate with about 20 moles of ethylene oxide	6
Ethanol	6
Dodecanamide	6

In all of the above formulations, other of the esters in the range hereinbefore delineated may be substituted for the ones mentioned either in a single compound form or at the blends derived from such natural sources as coconut oil. Substitution of higher molecular weight esters results in oilier products, while substitution of lower molecular weight esters results in less oily products. Use of esters beyond the essentially C₁₄-C₁₄ ester results in a very thick

product which also tends to increase the problem of the bathtub ring. Below the essentially C_8-C_8 ester, the product loses therapeutic and emollient value.

Additionally, any of the hereinbefore described oils, nonionic surface active agents or alcohols may be substituted in the examples in accordance with this invention. Perfumes and color are added to suit individual taste, but they affect this invention only by adding aesthetic appeal.

The foregoing description of the invention has been presented describing certain operable and preferred embodiments. It is not intended that the invention should be limited since variations and modifications thereof will be obvious to those skilled in the art, all of which are within the spirit and scope of this invention.

What is claimed is:

1. A clear, non-aqueous liquid composition containing 60% by weight of octyl dodecanoate, 30% by weight of light white mineral oil and 10% by weight of benzyl alcohol.

2. A clear, non-aqueous liquid composition containing 50% by weight of octyl dodecanoate, 37% by weight of light white mineral oil, 6% by weight of the condensation product of nonyl phenol with about 9.5 moles of ethylene oxide and 7% by weight of ethanol.

3. A clear, non-aqueous liquid composition containing 46% by weight of octyl dodecanoate, 35% by weight of light white mineral oil, 7% by weight of the condensa-

tion product of nonyl phenol with about 9.5 moles of ethylene oxide, 6% by weight of ethanol, and 6% by weight of N,N-diethanolododecanamide.

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ALBERT T. MEYERS, *Primary Examiner*.

D. R. MAHANAND, *Assistant Examiner*.