

Candidate's answer

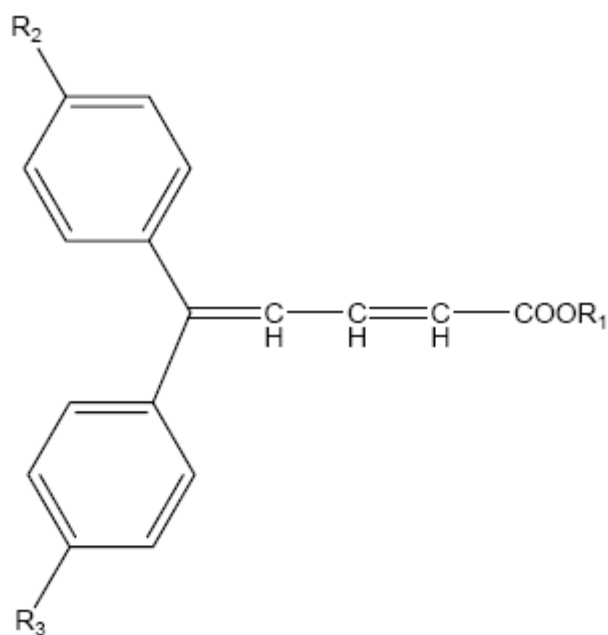
DESCRIPTION

The present invention relates to new UV-filters, method of producing the same and their use in cosmetic compositions, in particular sunscreens.

Sunscreens are cosmetic compositions that absorb UV radiation. This is commonly achieved by a combination of UV-A and UV-B filters. However, a known problem with conventional sunscreens is that the filters interact with each other. This renders the sunscreen compositions unstable with the result that their protective properties are considerably diminished over time.

In recent years, research has been carried out into UV-filters with improved stability. In this respect, the substitution with hydrophilic groups in known UV-filter compounds resulted in more stable sunscreens. Such compounds are soluble in water and, as a result, are easily removed from skin during bathing or perspiration.

For example, in D1 diarylbutadiene derivatives of the following formula were disclosed



wherein

R1 represents C1-C4-alkyl which may be substituted with OH, NH₂ or COOH, and

R2 and R3 independently from each other represent H, C1-C4-alkyl, halogen, Si(CH₃)₃, OH or NH₂;

as well as use of such compounds as UV-A filters in cosmetic compositions.

The compounds disclosed in D2 showed good photostability of 80% or higher and absorbed in the UV-A range. In some of the preferred compounds of D2 R1 was substituted with OH, NH₂, or COOH, increasing the hydrophilic character of R1. The compounds of D2 were reported to be useful in particular for the manufacture of cosmetic products having lighter and less oily feel such as daily-use cosmetic moisturizers.

In another prior art document, D1, other group of diarylbutadienes was described, depicted by the same general formula as the compounds of D2 but with the substituents of the following meaning:

R1 = C3-C10-cycloalkyl or phenyl, and

R2 and R3 independently from each other representing H, C1-C4-alkyl, halogen, Si(CH₃)₃, OH or NH₂.

The compounds disclosed in D1 have been found to constitute good comonomers to be copolymerised with styrene so as to obtain rubbery polymers with good abrasion properties and good performance at high temperatures.

As mentioned above UV-filters with improved stability, such as these described in D2 are soluble in water and are easily removed from the skin during bathing or perspiration.

Sunscreens are most commonly used to protect skin from excessive UV radiation. Exposure of the skin to such radiation very often takes place when it is relatively hot outside or in conditions where skin is also exposed to water. At high temperatures e.g. in the summer, when sunbathing is most popular skin easily becomes covered with sweat, which can remove UV-filters and thus reduce the effective UV-protection. In many summer and/or water sports such as yachting, surfing or swimming skin is also exposed both to UV-radiation and water.

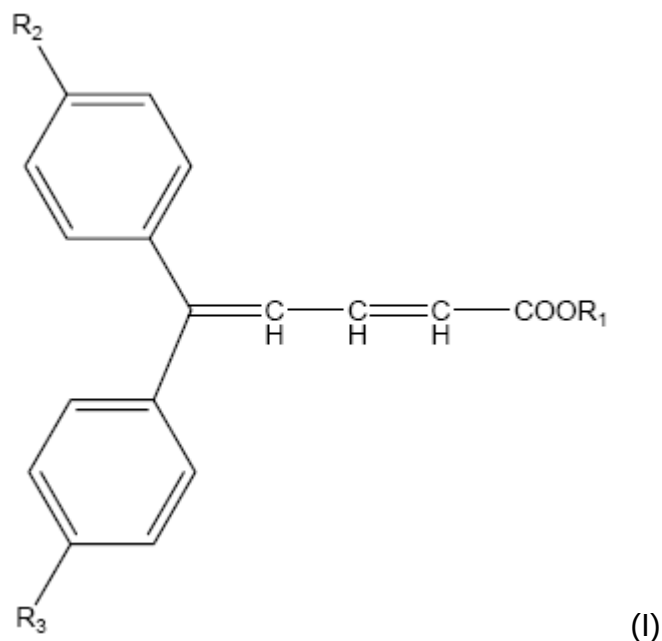
Taking into account the fact that in the situation described above sufficient and continuous protection against excessive UV-radiation is extremely important it was desired to provide UV-A filters that in addition to good photostability and other properties required in cosmetics applied directly to human skin showed good resistance to removal by water, in particular sweat, fresh water or sea water.

It has been now found that the compounds as defined in claim 1-3 are capable of providing all these requirements.

Further, the compounds of formula IA as defined in claim 8, wherein R1 represents C3-C10-cycloalkyl or phenyl

CLAIMS

A 4,4-diarylbutadiene derivative of formula (I):



wherein

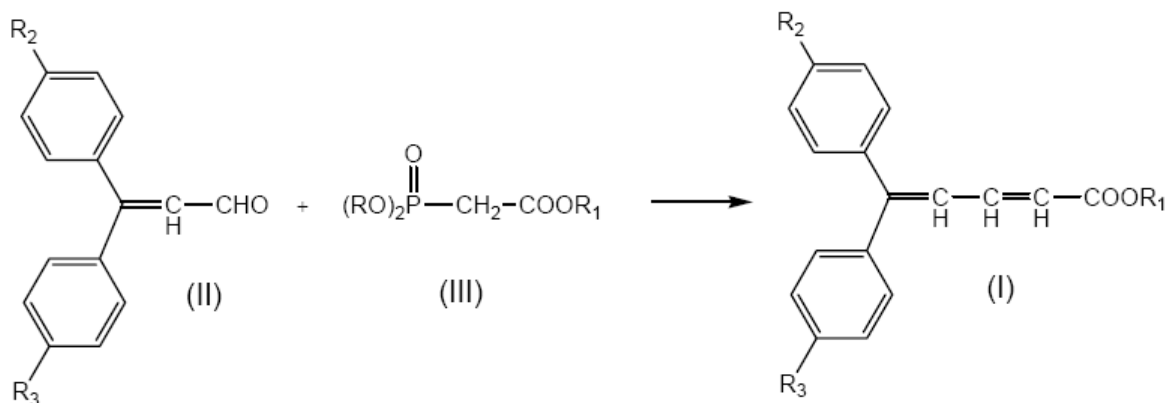
R1 represents alkyl containing at least 6 carbon atoms;

and either R2 or R3 represents Si(CH₃)₃ and the other one is selected from H, C1-C20-alkyl, halogen, Si(CH₃)₃, OH or NH₂.

The compound according to claim 1, wherein both R2 and R3 represent Si(CH₃)₃ groups.

The compound according to claim 1 or 2, wherein R1 represents heptyl, octyl or decyl.

A method for producing 4,4-diarylbutadiene derivatives of formula (I) as defined in claim 1, wherein a compound of formula (II) is reacted with a compound of formula (III),



wherein R is C1-C10-alkyl or phenyl,

and R1, R2 and R3 have the same meaning as defined in claim 1 in the presence of a base.

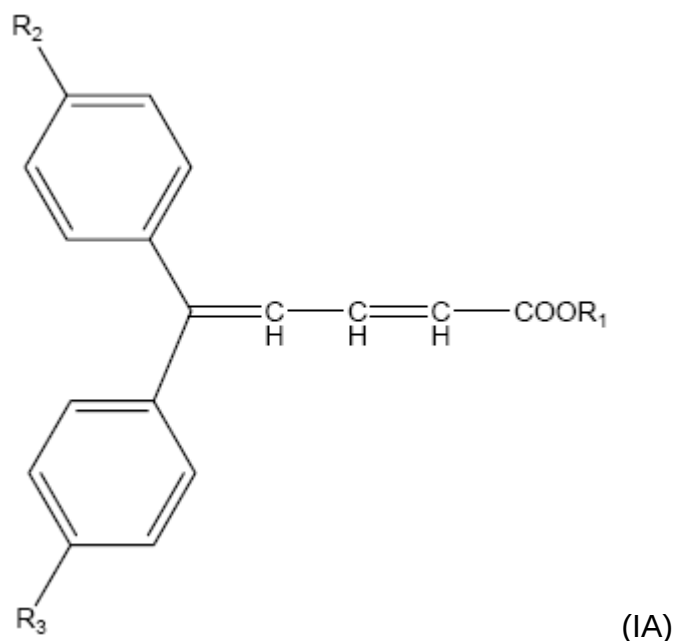
The method according to claim 4, wherein the compound of formula (III) is first mixed with a solvent at 0°C, then the base is added, subsequently the compound of formula (II) is slowly added and the reaction mixture is stirred for 1-2 hours at room temperature.

The method according to claim 4 or 5, wherein ethers are used as the solvent.

The method according to any of the claims 4 – 6, wherein LiOH is used as the base.

A sunscreen composition comprising

a 4,4-diarylbutadiene derivative of formula (IA)



wherein

R1 represents alkyl containing at least 6 carbon atoms, C3-C10-cycloalkyl or phenyl;
and

and either R2 or R3 represents Si(CH₃)₃ and the other one is selected from H, C1-C20-alkyl, halogen, Si(CH₃)₃, OH or NH₂;

in an amount of from 0.01 to 20 wt. % relative to the total weight of the composition;

at least one oil phase;

and further additives in amount of 1-80 wt.% relative to the total weight of the composition.

The sunscreen composition according to claim 8, comprising the compound of formula (IA) wherein both R2 and R3 represent Si(CH₃)₃ groups.

The sunscreen composition according to claim 8 or 9 in form of emulsion comprising an emulsifier.

The sunscreen composition according to claim 10 in form of a water-in-oil emulsion.

The sunscreen composition according to the claims 10 or 11, wherein the emulsifier is selected from sesquioleates, ethoxylated esters and polysiloxanes.

The sunscreen composition according to any of the claims 8-12, further comprising other UV-A filters and/or UV-B filters selected from salicylic acid, camphor, benzophenone and p-aminobenzoic acid.

The sunscreen composition according to any of the claims 8-13, wherein the additives include stabilizers, thickeners and/or preservatives.

Use of the 4,4-diarylbutadiene derivative of formula (IA) as defined in claim 8 for the manufacture of cosmetic compositions, in particular sunscreens.

EXAMINATION COMMITTEE I

Candidate No.

Paper A (Chemistry) 2012 - Marking Sheet

Category		Maximum possible	Marks awarded	
			Marker	Marker
Independent claims	Compound	30	30	30
	Compound for use	10	8	8
	Composition	20	15	15
	Process	10	10	10
Dependent claims		15	13	13
Description		15	7	7
Total		100	83	83

Examination Committee I agrees on 83 marks and recommends the following grade to the Examination Board:

☒ PASS
(50-100)

☐ COMPENSABLE FAIL
(45-49)

☐ FAIL
(0-44)

28 June 2012

Chairman of Examination Committee I