

DESCRIPTION

FRAGRANCE COMPOSITION

5 Technical Field

[0001] The present invention relates to a fragrance composition.

Background Art

[0002] Ethyl 2-cyclohexylpropionate has a fruity fragrance note, and is known as,
10 e.g., POIRENATE (Trade name of Kao Corporation).

[0003] A composition containing a cyclohexylpropanol derivative is known (see
Patent Document 1). This composition can be used for various products such as
fragrance compositions, perfumes, and shampoos.

[0004] A composition containing 2-(alkylcyclohexyl)-1-propanol is known (see Patent
15 Document 2). This 2-(alkylcyclohexyl)-1-propanol can provide a woody, floral
fragrance when it is, as a perfume substance, formulated into a usual fragrance.

[0005] A composition containing 1,1-(2,6,6-trimethylcyclohexyl)-hexan-3-ol is known
(see Patent Document 3). The addition of this substance brings about a rounding-off
and fixation of fragrance compositions while simultaneously increasing the intensity of
20 the fragrance.

[0006] A composition containing phenylalkanol is known (see Patent Document 4).
This phenylalkanol is suitable for perfuming, e.g., detergents, cleaners, textiles, and
plastic products because of its high stability to air and alkalis.

25 Prior Art Documents

Patent Documents

[0007] Patent Document 1: JP H03-66637 A

Patent Document 2: JP H01-207251 A

Patent Document 3: JP S54-117439 A

30 Patent Document 4: JP H01-503536 A

Disclosure of Invention

Problem to be Solved by the Invention

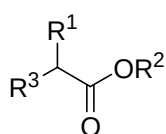
[0008] As described above, a fragrance composition containing a cyclohexylpropanol derivative or a compound having a similar structure is known. It is an object of the present invention to provide a new fragrance composition containing a 2-cycloalkylpropionate analogue.

Means for Solving Problem

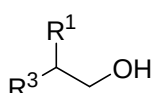
[0009] Surprisingly, the present inventors found that a composition in which 2-cycloalkylpropionate and 2-cycloalkylpropanol were combined demonstrated a good evaluation since the composition provided ester-like freshness and good emanation of scent. Based on the findings, the present inventors achieved a fragrance composition of the present invention.

[0010] That is, the present invention relates to a fragrance composition comprising a compound represented by Formula (1) (which may be hereinafter referred to as a “compound of Formula (1)” or “compound (1)”) and a compound represented by Formula (2) (which may be hereinafter referred to as a “compound of Formula (2)” or “compound (2)”), wherein a mass ratio of the compound represented by Formula (1) to the compound represented by Formula (2) (the compound represented by Formula (1) : the compound represented by Formula (2)) is 50:1 or more and 1999:1 or less.

[0011] [Chemical Formula 1]



(1)



(2)

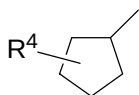
[0012] In Formula (1) and Formula (2),

R¹ is a hydrogen atom or an alkyl group with 1 or more and 3 or less of carbon atoms,

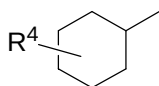
R² is an alkyl group with 1 or more and 4 or less of carbon atoms, and

R³ is a group represented by Formula (i) or Formula (ii) below.

[0013] [Chemical Formula 2]



(i)

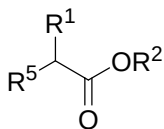


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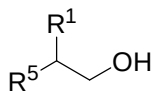
[0014] In Formula (i) and Formula (ii), R⁴ is a hydrogen atom or an alkyl group with 1 or more and 4 or less of carbon atoms.

[0015] In addition, the present invention relates to a method for manufacturing a
 5 fragrance composition that comprises adding hydrogen to a mixture containing a
 compound represented by Formula (3) (which may be hereinafter referred to as a
 “compound of Formula (3)” or “compound (3)”) and a compound represented by
 Formula (4) (which may be hereinafter referred to as a “compound of Formula (4)” or
 “compound (4)”) to obtain the composition containing the compound represented by
 10 Formula (1) and the compound represented by Formula (2).

[0016] [Chemical Formula 3]



(3)



(4)

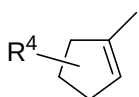
[0017] In Formula (3) and Formula (4),

15 R¹ is a hydrogen atom or an alkyl group with 1 or more and 3 or less of carbon
 atoms,

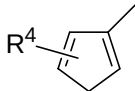
R² is an alkyl group with 1 or more and 4 or less of carbon atoms, and

R⁵ is any one of groups represented by Formulae (iii) to (viii) below.

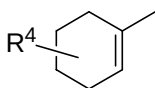
[0018] [Chemical Formula 4]



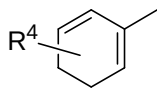
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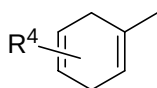
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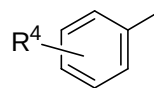
(v)



(vi)



(vii)



(viii)

[0019] In Formulae (iii) to (viii), R⁴ is a hydrogen atom or an alkyl group with 1 or more and 4 or less of carbon atoms.

Effects of the Invention

- 5 [0020] The present invention can provide a fragrance composition that provides ester-like freshness and good emanation of scent.

Description of the Invention

- [0021] As described above, the present invention relates to a fragrance composition
10 comprising a compound of Formula (1) and a compound of Formula (2), and in the fragrance composition, the mass ratio of the compound represented by Formula (1) to the compound represented by Formula (2) (the compound represented by Formula (1) : the compound represented by Formula (2)) is 50:1 or more and 1999:1 or less.

[0022] [Chemical Formula 5]



- 15 (1) (2)

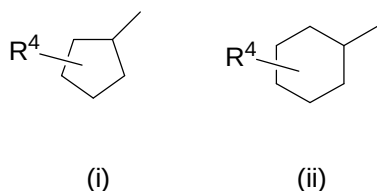
[0023] In Formula (1) and Formula (2),

R¹ is a hydrogen atom or an alkyl group with 1 or more and 3 or less of carbon atoms,

R² is an alkyl group with 1 or more and 4 or less of carbon atoms, and

- 20 R³ is a group represented by Formula (i) or Formula (ii) below.

[0024] [Chemical Formula 6]



[0025] In Formula (i) and Formula (ii), R⁴ is a hydrogen atom or an alkyl group with 1 or more and 4 or less of carbon atoms.

- 25 [0026] [Fragrance composition]

In the compound of Formula (1) and the compound of Formula (2), R¹ is

preferably alkyl with 1 or more and 3 or less of carbon atoms. Examples of the “alkyl group with 1 or more and 3 or less of carbon atoms” of R^1 include methyl, ethyl, n-propyl, i-propyl and the like. From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, the “alkyl group with 1 or more and 3 or less of carbon atoms” of R^1 is preferably methyl or ethyl, and more preferably methyl.

[0027] Examples of the “alkyl group with 1 or more and 4 or less of carbon atoms” of R^2 and R^4 in the compound of Formula (1) and the compound of Formula (2) include methyl, ethyl, n-propyl, i-propyl, n-butyl, sec-butyl, isobutyl, t-butyl and the like.

10 [0028] From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, the “alkyl group with 1 or more and 4 or less of carbon atoms” of R^2 is preferably methyl or ethyl, and more preferably ethyl.

[0029] From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, the “a hydrogen atom or an alkyl group with 1 or more and 4 or less of carbon atoms” of R^4 is preferably a hydrogen atom, methyl, or ethyl, more preferably a hydrogen atom or methyl, and further preferably hydrogen.

15 [0030] As described above, R^3 in the compound of Formula (1) and the compound of Formula (2) is a group represented by Formula (i) or Formula (ii). From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, R^3 is preferably a group represented by Formula (ii).

[0031] From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, in the fragrance composition of the present invention, the mass concentration of the compound of Formula (1) is preferably 90% by mass or more, more preferably 93% by mass or more, and further preferably 96% by mass or more, and preferably 99.95% by mass or less, more preferably 99.93% by mass or less, and further preferably 99.90% by mass or less.

25 [0032] From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, in the fragrance composition of the present invention, the mass concentration of the compound of Formula (2) is preferably 500 ppm or more, more preferably 700 ppm or more, and further preferably 900 ppm or more, and preferably 15000 ppm or less, more preferably 8000 ppm or less, further preferably 5000 ppm or less, and still further preferably 3000 ppm or less.

[0033] From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, in the fragrance composition of the present invention, the mass ratio of the compound of Formula (1) to the compound of Formula (2) (the compound of Formula (1) : the compound of Formula (2)) is 50:1 or more, preferably 120:1 or more, more preferably 300:1 or more, and further preferably 600:1 or more, and 1999:1 or less, preferably 1600:1 or less, and more preferably 1350:1 or less.

[0034] In the fragrance composition of the present invention, the compound of Formula (1) is preferably methyl 2-cyclohexylbutanoate, ethyl 2-cyclohexylbutanoate, methyl 2-cyclopentylpropionate, ethyl 2-cyclopentylpropionate, isopropyl 2-cyclopentylpropionate, methyl 2-cyclohexylpropionate, ethyl 2-cyclohexylpropionate, isopropyl cyclohexylacetate, methyl cyclohexylacetate, ethyl cyclohexylacetate, or isopropyl cyclohexylacetate; more preferably methyl 2-cyclopentylpropionate, ethyl 2-cyclopentylpropionate, methyl 2-cyclohexylpropionate, ethyl 2-cyclohexylpropionate, isopropyl cyclohexylacetate, methyl cyclohexylacetate, or ethyl cyclohexylacetate; and further preferably methyl 2-cyclohexylpropionate, ethyl 2-cyclohexylpropionate, methyl cyclohexylacetate, or ethyl cyclohexylacetate. The compound of Formula (2) is preferably 2-cyclopentylbutanol, 2-cyclopentylpropanol, 2-cyclohexylpropanol, or cyclohexylethanol, more preferably 2-cyclohexylpropanol or 2-cyclohexylethanol, and further preferably 2-cyclohexylethanol.

[0035] In the fragrance composition of the present invention, the following combinations of the compound of Formula (1) and the compound of Formula (2) are preferred.

[0036] [Table 1]

	Compound of Formula (1)	Compound of Formula (2)
Combination i	Ethyl 2-cyclohexylpropionate	2-cyclohexylpropanol
Combination ii	Methyl 2-cyclohexylpropionate	2-cyclohexylpropanol
Combination iii	Ethyl cyclohexylacetate	2-cyclohexylethanol
Combination iv	Methyl cyclohexylacetate	2-cyclohexylethanol

[0037] The fragrance composition of the present invention can be used in combination with other fragrances.

[0038] The fragrance composition of the present invention provides ester-like freshness and good emanation of scent as a fragrance, and thus can be used as a

fragrance material.

[0039] The present invention further provides a cleaner containing the fragrance composition of the present invention, a cosmetic containing the fragrance composition of the present invention, and a fiber treating agent containing the fragrance composition of the present invention.

[0040] The cleaner of the present invention is preferably a body cleaner, a cleaner for clothing, or a cleaner for hard surfaces, more preferably a body cleaner or a cleaner for clothing, and further preferably a cleaner for clothing.

[0041] Examples of the body cleaner include a skin cleaner, a hair cleaner, and a soap. The body cleaner is preferably a skin cleaner.

[0042] Examples of the cleaner for hard surfaces include an all purpose cleaner and a cleaner for tableware.

[0043] The fiber treating agent of the present invention is preferably a softener.

[0044] The cosmetic of the present invention is preferably a perfume, a milky lotion, a skin lotion, or a sunscreen, and more preferably a perfume.

[0045] The cleaner of the present invention preferably contains an anionic surfactant other than the fragrance composition of the present invention. The cleaner may further contain a nonionic surfactant, a pH adjuster, a viscosity modifier, a solvent, an oil, an antiseptic agent, water, or the like.

[0046] The fiber treating agent of the present invention preferably contains a cationic surfactant other than the fragrance composition of the present invention. The fiber treating agent may further contain a pH adjuster, a solvent, an oil, an antiseptic agent, water, or the like.

[0047] The perfume of the present invention may contain a solvent, water, or the like other than the fragrance composition of the present invention.

[0048] The fragrance composition of the present invention is contained preferably in an amount of 0.00001% by mass or more, and more preferably in an amount of 0.0001% by mass or more, and preferably in an amount of 0.01% by mass or less, and more preferably in an amount of 0.001% by mass or less based on the cleaner, the cosmetic, or the softener. It is possible to provide ester-like freshness and good emanation of scent by using the fragrance composition in this amount.

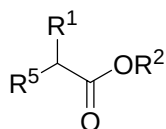
[0049] The fragrance composition of the present invention is contained preferably in

an amount of 0.0001% by mass or more, and more preferably in an amount of 0.001% by mass or more and preferably in an amount of 0.1% by mass or less, and more preferably in an amount of 0.01% by mass or less based on the perfume. It is possible to provide ester-like freshness and good emanation of scent by using the fragrance composition in this amount.

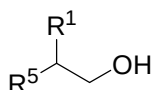
[0050] <Method for manufacturing fragrance composition>

In addition, the present invention relates to a method for manufacturing a fragrance composition that comprises adding hydrogen to a mixture containing a compound of Formula (3) and a compound of Formula (4) (also simply referred to as a “raw material composition”) to obtain the composition containing the compound represented by Formula (1) and the compound represented by Formula (2).

[0051] [Chemical Formula 7]



(3)



(4)

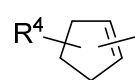
[0052] In Formula (3) and Formula (4),

R¹ is a hydrogen atom or an alkyl group with 1 or more and 3 or less of carbon atoms,

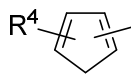
R² is an alkyl group with 1 or more and 4 or less of carbon atoms, and

R⁵ is any one of groups represented by Formulae (iii) to (viii) below.

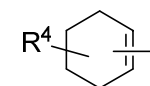
[0053] [Chemical Formula 8]



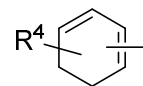
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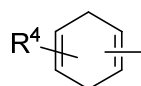
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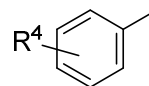
(v)



(vi)



(vii)



(viii)

[0054] In Formulae (iii) to (viii), R⁴ is a hydrogen atom or an alkyl group with 1 or more and 4 or less of carbon atoms.

[0055] In accordance with the manufacturing method, the compound of Formula (1) is obtained by adding hydrogen to the compound of Formula (3), and the compound of Formula (2) is obtained by adding hydrogen to the compound of Formula (4).

[0056] [Compound of Formula (3) and compound of Formula (4)]

5 In the compound of Formula (3) and the compound of Formula (4), R¹ is preferably an alkyl group with 1 or more and 3 or less of carbon atoms. Examples of the “alkyl group with 1 or more and 3 or less of carbon atoms” of R¹ include methyl, ethyl, n-propyl, i-propyl and the like. From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, the “alkyl group
10 with 1 or more and 3 or less of carbon atoms” of R¹ is preferably methyl or ethyl, and more preferably methyl.

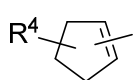
[0057] Examples of the “alkyl group with 1 or more and 4 or less of carbon atoms” of R² and R⁴ in the compound of Formula (3) and the compound of Formula (4) include methyl, ethyl, n-propyl, i-propyl, n-butyl, sec-butyl, isobutyl, t-butyl and the like.

15 [0058] From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, the “alkyl group with 1 or more and 4 or less of carbon atoms” of R² is preferably methyl or ethyl, and more preferably ethyl.

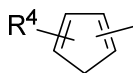
[0059] From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, the “a hydrogen atom or an alkyl group with 1 or
20 more and 4 or less of carbon atoms” of R⁴ is preferably a hydrogen atom, methyl, or ethyl, more preferably a hydrogen atom or methyl, and further preferably a hydrogen atom.

[0060] As described above, R⁵ in the compound of Formula (3) and the compound of Formula (4) is any one of groups represented by Formulae (iii) to (viii). From the
25 viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, R⁵ is preferably any one of groups represented by Formulae (v) to (viii), and more preferably a group represented by Formula (viii).

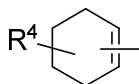
[0061] [Chemical Formula 9]



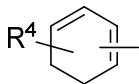
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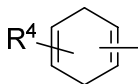
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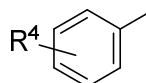
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(viii)

[0062] As described above, R^4 in R^5 of the compound of Formula (3) and the compound of Formula (4) is a hydrogen atom or an alkyl group with 1 or more and 4 or less of carbon atoms. From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, R^4 is preferably a hydrogen atom or a methyl group.

[0063] To obtain the fragrance composition in which the mass ratio of the compound of Formula (1) to the compound of Formula (2) is 50:1 or more and 1999:1 or less, it is preferable to set the mass ratio of the compound represented by Formula (3) to the compound represented by Formula (4) within a predetermined range in adding hydrogen to the compound of Formula (3) and the compound of Formula (4) that are raw materials.

[0064] From the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, in adding hydrogen to the compound of Formula (3) and the compound of Formula (4), the mass ratio of the compound represented by Formula (3) to the compound represented by Formula (4) is preferably 50:1 or more, more preferably 120:1 or more, further preferably 300:1 or more, and still further preferably 600:1 or more, and preferably 1999:1 or less, more preferably 1600:1 or less, and further preferably 1350:1 or less.

[0065] In addition, from the viewpoint of causing ester-like freshness and good emanation of scent of the fragrance composition, in adding hydrogen to the compound of Formula (3) and the compound of Formula (4), the mass concentration of the compound represented by Formula (4) in the raw material composition is preferably 100 ppm or more, more preferably 200 ppm or more, and further preferably 250 ppm

or more, and preferably 2500 ppm or less, more preferably 1600 ppm or less, and further preferably 1000 ppm or less.

[0066] The step of adding hydrogen to the compound of Formula (3) and the compound of Formula (4) is performed by reacting them with hydrogen in the presence of a catalyst. Examples of an active metal species in the catalyst include nickel, platinum, palladium, ruthenium, rhodium and the like. From the viewpoint of the efficiency of hydrogenation reaction, the active metal species is preferably platinum, palladium, ruthenium, or rhodium, more preferably platinum or ruthenium, and further preferably ruthenium.

[0067] The amount of the active metal in the catalyst to be used is preferably 0.001 to 1% by mass, more preferably 0.01 to 0.5% by mass, and further preferably 0.02 to 0.2% by mass based on the total of the compound of Formula (3) and the compound of Formula (4).

[0068] The step of adding hydrogen to the compound of Formula (3) and the compound of Formula (4) is performed, e.g., under a hydrogen pressure of 10 to 200 MPa. From the viewpoint of the efficiency of hydrogenation reaction, the hydrogen pressure is preferably 1.0 to 20 MPa, and more preferably 1.5 MPa to 5.0 MPa.

[0069] The step of adding hydrogen to the compound of Formula (3) and the compound of Formula (4) is performed, e.g., at a temperature of 80°C to 200°C. From the viewpoint of the efficiency of hydrogenation reaction, the temperature is preferably 100°C to 200°C, and more preferably 120°C to 180°C.

[0070] From the viewpoint of providing the fragrance composition of the present invention, in the manufacturing method of the present invention, the mass concentration of the compound of Formula (3) in the raw material composition is preferably 90% by mass or more, more preferably 95% by mass or more, and further preferably 98% by mass or more, and preferably 99.99% by mass or less, more preferably 99.96% by mass or less, and further preferably 99.93% by mass or less.

[0071] From the viewpoint of providing the fragrance composition of the present invention, in the manufacturing method of the present invention, the mass concentration of the compound of Formula (4) in the raw material composition is preferably 150 ppm or more, more preferably 200 ppm or more, and further preferably 250 ppm or more, and preferably 2500 ppm or less, more preferably 1600 ppm or less,

and further preferably 1000 ppm or less.

[0072] From the viewpoint of providing the fragrance composition of the present invention, in the manufacturing method of the present invention, the mass ratio of the compound of Formula (3) to the compound of Formula (4) (the compound of Formula (3) : the compound of Formula (4)) is preferably 500:1 or more, more preferably 650:1 or more, and further preferably 1000:1 or more, and preferably 10000:1 or less, more preferably 7000:1 or less, and further preferably 4500:1 or less.

[0073] The step of adding hydrogen to the mixture of the compound of Formula (3) and the compound of Formula (4) is performed, e.g., for 2 to 24 hours, preferably for 3 to 20 hours, and more preferably for 4 to 12 hours from the viewpoint of providing the fragrance composition of the present invention.

[0074] The step of adding hydrogen to the mixture of the compound of Formula (3) and the compound of Formula (4) is performed, e.g., under a hydrogen pressure of 10 to 200 MPa at a temperature of 80°C to 200°C for 2 to 24 hours. From the viewpoint of the efficiency of hydrogenation reaction, the adding is performed preferably under a hydrogen pressure of 1.0 to 20 MPa at a temperature of 100°C to 200°C for 3 to 20 hours, and more preferably under a hydrogen pressure of 1.5 MPa to 5.0 MPa at a temperature of 120°C to 180°C for 4 to 12 hours.

[0075] After hydrogenation of the compound of Formula (3) and the compound of Formula (4) and purification by a usual method, the composition comprising the compound of Formula (1) and the compound of Formula (2) can be obtained. The usual method is a purification method in which distillation under reduced pressure and column chromatography may be used.

[0076] In the fragrance composition of the present invention, the compound of Formula (3) is preferably methyl 2-phenylbutanoate, ethyl 2-phenylbutanoate, methyl 2-cyclopentenylpropionate, ethyl 2-cyclopentenylpropionate, isopropyl 2-cyclopentenylpropionate, methyl 2-phenylpropionate, ethyl 2-phenylpropionate, isopropyl phenylacetate, methyl phenylacetate, ethyl phenylacetate, or isopropyl phenylacetate; more preferably methyl 2-cyclopentenylpropionate, ethyl 2-cyclopentenylpropionate, methyl 2-phenylpropionate, ethyl 2-phenylpropionate, isopropyl phenylacetate, methyl phenylacetate, or ethyl phenylacetate; and further preferably methyl 2-phenylpropionate, ethyl 2-phenylpropionate, methyl

phenylacetate, or ethyl phenylacetate. The compound of Formula (4) is preferably 2-phenylbutanol, 2-cyclopentenylpropanol, 2-phenylpropanol, or phenylethanol, and more preferably 2-phenylpropanol or 2-phenylethanol.

[0077] In the manufacturing method of the present invention, the following

5 combinations of the compound of Formula (3) and the compound of Formula (4) are preferred.

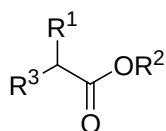
[0078] [Table 2]

	Compound of Formula (3)	Compound of Formula (4)
Combination i	Ethyl 2-phenylpropionate	2-phenylpropanol
Combination ii	Methyl 2-phenylpropionate	2-phenylpropanol
Combination iii	Ethyl phenylacetate	2-phenylethanol
Combination iv	Methyl phenylacetate	2-phenylethanol

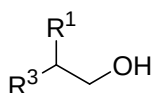
[0079] With regard to the embodiment described above, the present invention further discloses the following fragrance composition and manufacturing method thereof.

10 [0080] <1> A fragrance composition comprising a compound represented by Formula (1) and a compound represented by Formula (2), wherein a mass ratio of the compound represented by Formula (1) to the compound represented by Formula (2) (the compound represented by Formula (1) : the compound represented by Formula (2)) is 50:1 or more and 1999:1 or less,

15 [0081] [Chemical Formula 10]



(1)



(2)

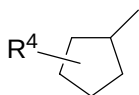
[0082] wherein, in Formula (1) and Formula (2),

R¹ is a hydrogen atom or an alkyl group with 1 or more and 3 or less of carbon atoms,

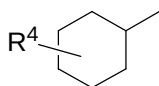
20 R² is an alkyl group with 1 or more and 4 or less of carbon atoms, and

R³ is a group represented by Formula (i) or Formula (ii) below,

[0083] [Chemical Formula 11]



(i)



(ii)

[0084] wherein, in Formula (i) and Formula (ii), R⁴ is a hydrogen atom or an alkyl group with 1 or more and 4 or less of carbon atoms.

[0085] <2> The fragrance composition according to <1>, wherein, in the fragrance composition containing the compound represented by Formula (1) and the compound represented by Formula (2), a mass concentration of the compound represented by Formula (2) is 500 ppm or more and 15000 ppm or less.

[0086] <3> The fragrance composition according to <2>, wherein, in the fragrance composition containing the compound represented by Formula (1) and the compound represented by Formula (2), the mass concentration of the compound represented by Formula (2) is 700 ppm or more and 3000 ppm or less.

[0087] <4> The fragrance composition according to any one of <1> to <3>, wherein a mass concentration of the compound represented by Formula (1) is 90% by mass or more and 99.95% by mass or less.

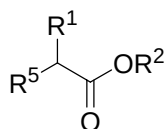
[0088] <5> The fragrance composition according to <4>, wherein the mass concentration of the compound represented by Formula (1) is 96% by mass or more and 99.90% by mass or less.

[0089] <6> The fragrance composition according to any one of <1> to <5>, wherein, in Formula (1) and Formula (2), R³ is a group represented by Formula (ii).

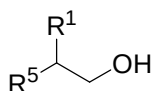
[0090] <7> The fragrance composition according to any one of <1> to <6>, wherein R⁴ in Formula (1) and Formula (2) is a hydrogen atom or a methyl group.

[0091] <8> A method for manufacturing a fragrance composition, comprising adding hydrogen to a mixture comprising a compound represented by Formula (3) and a compound represented by Formula (4) to obtain the composition comprising the compound represented by Formula (1) and the compound represented by Formula (2),

[0092] [Chemical Formula 12]



(3)



(4)

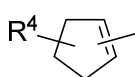
[0093] wherein, in Formula (3) and Formula (4),

R¹ is a hydrogen atom or an alkyl group with 1 or more and 3 or less of carbon atoms,

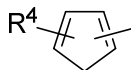
5 R² is an alkyl group with 1 or more and 4 or less of carbon atoms, and

R⁵ is any one of groups represented by Formulae (iii) to (viii) below,

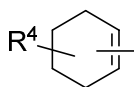
[0094] [Chemical Formula 13]



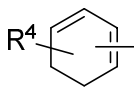
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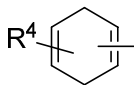
(iv)



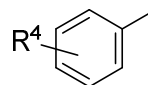
(v)



(vi)



(vii)



(viii)

[0095] wherein, in Formulae (iii) to (viii), R⁴ is a hydrogen atom or an alkyl group
10 with 1 or more and 4 or less of carbon atoms.

[0096] <9> The method according to <8>, wherein the mass ratio of the compound represented by Formula (1) to the compound represented by Formula (2) (the compound represented by Formula (1) : the compound represented by Formula (2)) is 50:1 or more and 1999:1 or less.

15 [0097] <10> The method according to <9>, wherein the mass ratio of the compound represented by Formula (1) and the compound represented by Formula (2) (the compound represented by Formula (1) : the compound represented by Formula (2)) is 300:1 or more and 1350:1 or less.

[0098] <11> The method according to any one of <8> to <10>, wherein, in the

20 mixture containing the compound represented by Formula (3) and the compound represented by Formula (4), a mass concentration of the compound represented by Formula (4) is 100 ppm or more and 2500 ppm or less.

[0099] <12> The method according to <11>, wherein, in the mixture containing the compound represented by Formula (3) and the compound represented by Formula (4), the mass concentration of the compound represented by Formula (4) is 200 ppm or more and 1000 ppm or less.

5 [0100] <13> The method according to any one of <8> to <12>, wherein, in Formula (3) and Formula (4), R⁵ is any one of groups represented by Formulae (v) to (viii).

[0101] <14> The method according to <13>, wherein, in Formula (3) and Formula (4), R⁵ is a group represented by Formula (viii).

10 [0102] <15> The method according to any one of <8> to <14>, wherein R⁴ in Formula (3) and Formula (4) is a hydrogen atom or a methyl group.

[0103] Details of the measurement methods performed in the following examples and the like are described together below.

[0104] In the examples and comparative example, the term “%” indicates “% by mass”, unless otherwise noted.

15 [0105] The following raw materials were used for reaction.

5% ruthenium supported on carbon powder: manufactured by N.E.

CHEMCAT Corporation

Ethyl 2-phenylpropionate: manufactured by Kuraray Co., Ltd.

2-phenylpropanol: manufactured by Tokyo Chemical Industry Co., Ltd.

20 2-propanol: manufactured by Wako Pure Chemical Industries, Ltd., Wako special grade

[0106] The composition of a reaction solution or a distillate was analyzed by gas chromatography. Specifically, a 0.1 mL portion of a filtrate obtained by filtrating the reaction solution or a 0.1 mL portion of the distillate was diluted in 1 mL of 2-propanol, and the resultant solution was measured by gas chromatography. A ratio between peak areas derived from components in chromatogram obtained as a result of the measurement was defined as a mass ratio between the components.

[0107] <Apparatus and analytical conditions for gas chromatography (GC)>

30 GC apparatus: 7890B manufactured by Agilent Technologies, Inc., flame ionization detector

Column: DB-1 (capillary column, 100% dimethylpolysiloxane, inner diameter: 0.25 mm, length: 30 m, and film thickness: 0.25 μm) manufactured by Agilent

Technologies, Inc.

Carrier gas: He, 1.5 mL/min

Injection condition: 300°C, split ratio: 100/1

Injection Amount: 1 µL

5 Detection condition: FID System, 300°C

Column temperature condition: 80°C → Raised at 10°C/min → Maintained at 300°C for 10 minutes

[0108] <Identification of compound>

10 Identification was performed by gas chromatography using the following compounds as standards in the following examples and comparative example. The compounds were commercially available or separately produced in accordance with a known document.

[0109] Ethyl 2-phenylpropionate: manufactured by Kuraray Co., Ltd.

2-phenylpropanol: manufactured by Tokyo Chemical Industry Co., Ltd.

15 Ethyl 2-cyclohexylpropionate: "POIRENATE" (trade name) manufactured by Kao Corporation

2-cyclohexylpropanol: produced from 2-phenylpropionaldehyde in accordance with a method described in WO 2016/202253.

[0110] <Example 1>

20 After 4.2 g of 5% ruthenium supported on carbon powder (containing 55% water) as a catalyst was placed into a 500 mL autoclave made of a titanium alloy, 200 g of ethyl 2-phenylpropionate (containing 230 ppm of 2-phenylpropanol) was added thereto. After the autoclave was sealed, the hydrogen pressure was adjusted to 1.0 MPa, and stirring (500 rpm) and increasing the temperature (140°C) were started.

25 After the internal temperature reached 140°C, the hydrogen pressure was adjusted to 2.0 MPa, and hydrogenation reaction was performed at 2.0 MPa and 140°C for 6 hours. The resultant reaction solution was subjected to GC analysis after 6 hours. The GC analysis confirmed that 99.5% of the reaction solution was converted into ethyl 2-cyclohexylpropionate.

30 [0111] The reaction crude product thus obtained was filtrated using a filter paper (No. 5C manufactured by Advantech Co., Ltd.). A 150 g portion of the filtrate thus obtained was placed into a 300 mL Hertz flask and distilled under reduced pressure

using a rectifying column (inner diameter 28 mm × height 1000 mm, packing: Sulzer) at 4.0 kPa, 120°C to 140°C, and a reflux ratio of 1.0 to 10.0. As a main fraction, 134 g of a distillate was obtained. As a result of the GC analysis, it was confirmed that the distillate was a composition containing 99.90% ethyl 2-cyclohexylpropionate and 756 ppm of 2-cyclohexylpropanol. Table 1 indicates the obtained results.

[0112] <Example 2>

Example 2 was performed in the same manner as in Example 1 except that ethyl 2-phenylpropionate (containing 149 ppm of 2-phenylpropanol) was used instead of ethyl 2-phenylpropionate (containing 230 ppm of 2-phenylpropanol). Table 1 indicates the obtained results.

[0113] <Example 3>

Example 3 was performed in the same manner as in Example 1 except that ethyl 2-phenylpropionate (containing 252 ppm of 2-phenylpropanol) was used instead of ethyl 2-phenylpropionate (containing 230 ppm of 2-phenylpropanol). Table 1 indicates the obtained results.

[0114] <Example 4>

Example 4 was performed in the same manner as in Example 1 except that ethyl 2-phenylpropionate (containing 406 ppm of 2-phenylpropanol) was used instead of ethyl 2-phenylpropionate (containing 230 ppm of 2-phenylpropanol). Table 1 indicates the obtained results.

[0115] <Example 5>

Example 5 was performed in the same manner as in Example 1 except that ethyl 2-phenylpropionate (containing 1555 ppm of 2-phenylpropanol) was used instead of ethyl 2-phenylpropionate (containing 230 ppm of 2-phenylpropanol). Table 1 indicates the obtained results.

[0116] <Example 6>

Example 6 was performed in the same manner as in Example 1 except that ethyl 2-phenylpropionate (containing 2862 ppm of 2-phenylpropanol) was used instead of ethyl 2-phenylpropionate (containing 78 ppm of 2-phenylpropanol). Table 1 indicates the obtained results.

[0117] <Comparative Example 1>

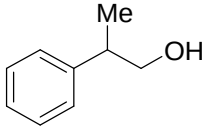
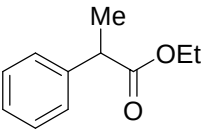
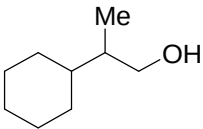
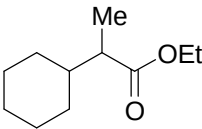
Comparative Example 1 was performed in the same manner as in Example 1

except that ethyl 2-phenylpropionate (containing 78 ppm of 2-phenylpropanol) was used instead of ethyl 2-phenylpropionate (containing 230 ppm of 2-phenylpropanol).

Table 1 indicates the obtained results.

[0118] [Table 3]

5 Table 1

	Raw material composition		Produced composition	
	2-phenylpropanol	Ethyl 2-phenylpropionate	2-cyclohexylpropanol	Ethyl 2-cyclohexylpropionate
				
	[ppm]	[%]	[ppm]	[%]
Ex. 1	230	99.95	756	99.90
Ex. 2	149	99.96	515	99.95
Ex. 3	252	99.96	962	99.88
Ex. 4	406	99.94	1561	99.82
Ex. 5	1555	99.82	5928	99.36
Ex. 6	2862	99.68	11463	98.82
Comp. Ex. 1	78	99.97	389	99.96

*Ex.: Example, Comp. Ex.: Comparative Example

[0119] [Sensory evaluation]

The odor of the composition produced in each of Examples 1 to 6 and Comparative Example 1 was evaluated with the average of two expert panelist. The evaluation was performed using a fragrance test paper having a size of 150 mm × 7 mm (manufactured by Daimonji Paper Co., Ltd.), 10 µl of each main fraction was imparted to the fragrance test paper at its end, and the evaluation was performed indoor after one hour. The evaluation was performed from the viewpoints of the intensity and the quality of the odor. The intensity was evaluated in 5 stages. The greater the value of the intensity was, the more preferable it was. Regarding the quality, a feature of the odor that was felt was described. Table 2 indicates the obtained results.

[0120] [Table 4]

Table 2

	Evaluation result	
	Intensity	Quality
Ex. 1	5	Particularly good since ester-like freshness and good emanation of scent were strongly felt.
Ex. 2	4.5	Good since ester-like freshness and good emanation of scent were felt.
Ex. 3	5	Particularly good since ester-like freshness and good emanation of scent were strongly felt.
Ex. 4	5	Particularly good since ester-like freshness and good emanation of scent were strongly felt.
Ex. 5	4.5	Good since ester-like freshness and good emanation of scent were felt.
Ex. 6	4	Ester-like freshness and emanation of scent were somewhat weak.
Comp. Ex. 1	3	Ester-like freshness and emanation of scent were somewhat weak.

*Ex.: Example, Comp. Ex.: Comparative Example

[0121] As indicated in Table 2, the compositions of the present invention demonstrated good evaluations since they provided ester-like freshness and good emanation of scent.

5

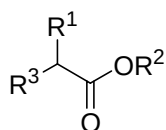
Industrial Applicability

[0122] The fragrance composition of the present invention provides ester-like freshness and good emanation of scent as a fragrance, and thus can be used as a fragrance material.

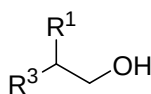
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CLAIMS

1. A fragrance composition comprising:
 a compound represented by Formula (1); and
 a compound represented by Formula (2),
 wherein a mass ratio of the compound represented by Formula (1) to the
 compound represented by Formula (2) (the compound represented by Formula (1) : the
 compound represented by Formula (2)) is 50:1 or more and 1999:1 or less
 [Chemical Formula 14]



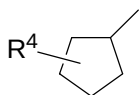
(1)



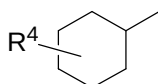
(2)

- wherein, in Formula (1) and Formula (2),
 R¹ is a hydrogen atom or an alkyl group with 1 or more and 3 or less of carbon
 atoms,
 R² is an alkyl group with 1 or more and 4 or less of carbon atoms, and
 R³ is a group represented by Formula (i) or Formula (ii) below

- [Chemical Formula 15]



(i)



(ii)

- wherein, in Formula (i) and Formula (ii), R⁴ is a hydrogen atom or an alkyl
 group with 1 or more and 4 or less of carbon atoms.
2. The fragrance composition according to claim 1, wherein in the fragrance
 composition comprising the compound represented by Formula (1) and the compound
 represented by Formula (2), a mass concentration of the compound represented by
 Formula (2) is 500 ppm or more and 15000 ppm or less.
3. The fragrance composition according to claim 1 or 2, wherein a mass
 concentration of the compound represented by Formula (1) is 90% by mass or more

and 99.95% by mass or less.

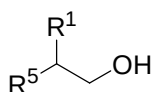
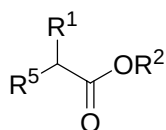
4. The fragrance composition according to any one of claims 1 to 3, wherein, in Formula (1) and Formula (2), R^3 is a group represented by Formula (ii).

5

5. The fragrance composition according to any one of claims 1 to 4, wherein R^4 in Formula (1) and Formula (2) is a hydrogen atom or a methyl group.

6. A method for manufacturing a fragrance composition, comprising:
 10 adding hydrogen to a mixture comprising a compound represented by Formula (3) and a compound represented by Formula (4) to obtain the composition comprising the compound represented by Formula (1) and the compound represented by Formula (2)

[Chemical Formula 16]



15

(3)

(4)

wherein, in Formula (3) and Formula (4),

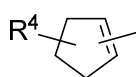
R^1 is a hydrogen atom or an alkyl group with 1 or more and 3 or less of carbon atoms,

R^2 is an alkyl group with 1 or more and 4 or less of carbon atoms, and

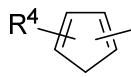
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R^5 is any one of groups represented by Formulae (iii) to (viii) below

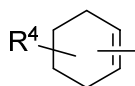
[Chemical Formula 17]



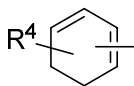
(iii)



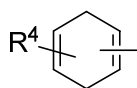
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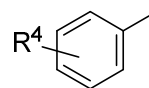
(v)



(vi)



(vii)



(viii)

wherein, in Formulae (iii) to (viii), R⁴ is a hydrogen atom or an alkyl group with 1 or more and 4 or less of carbon atoms.

7. The method according to claim 6, wherein the mass ratio of the compound
5 represented by Formula (1) to the compound represented by Formula (2) (the
compound represented by Formula (1) : the compound represented by Formula (2)) is
50:1 or more and 1999:1 or less.
8. The method according to claim 6 or 7, wherein, in the mixture comprising the
10 compound represented by Formula (3) and the compound represented by Formula (4),
a mass concentration of the compound represented by Formula (4) is 100 ppm or more
and 2500 ppm or less.
9. The method according to any one of claims 6 to 8 or claim 7, wherein, in
15 Formula (3) and Formula (4), R⁵ is any one of groups represented by Formulae (v) to
(viii).
10. The method according to any one of claims 6 to 9, wherein R⁴ in Formula (3)
and Formula (4) is a hydrogen atom or a methyl group.